An ICME Approach to Predicting Chemistry and Process Specific Localized Precipitation Behavior During Additive Manufacturing by Linking Finite Element Tools to Computational Thermodynamics

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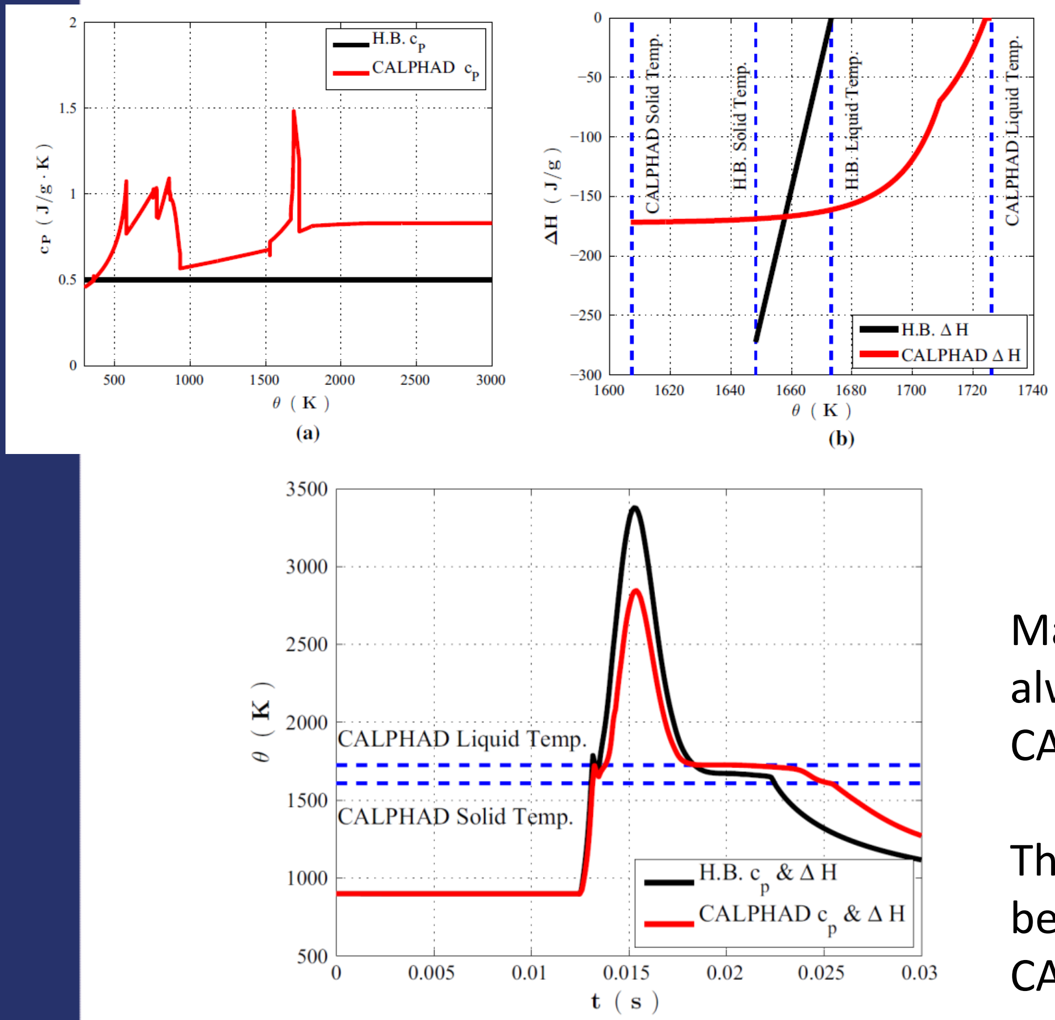
Outline

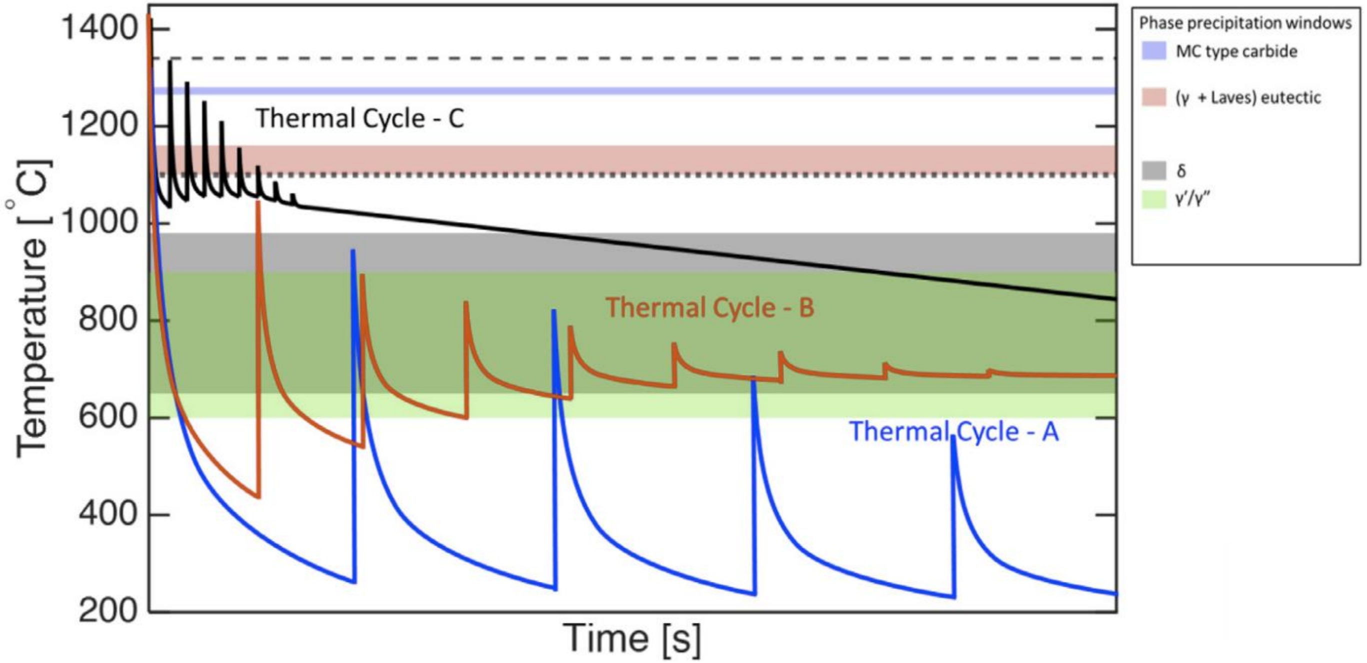
- Inspiration for this ICME framework
- Details of this work
- Calphad background
- FEM simulations
    - LPBF
    - EBD
    - WAAM
- Precipitation simulations
- Assumptions/Future work

Thermo-Calc Software

Inspiration



Smith, et al. / *Computational Mechanics* 57.4 (2016): 583-610.

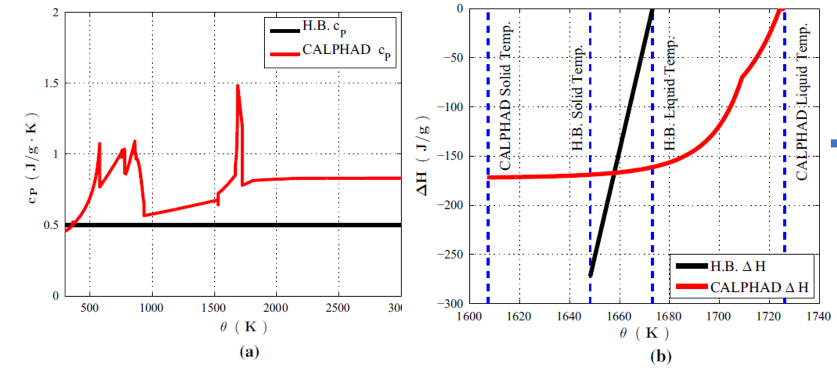


Kumara, Chamara, et al. *Additive Manufacturing* 25 (2019): 357-364.

Material property data as a function of temperature not always available in literature/handbooks

CALPHAD calculated data can improve models (Smith, et al.)

Thermal cycling during building influences precipitation behavior (Kumara, et al.)– thermal data can be fed into CALPHAD to predict this



CALPHAD

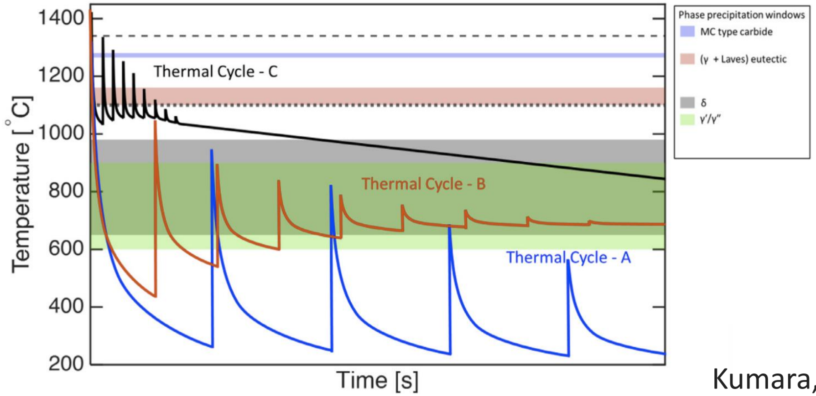
Smith, et al. / *Computational Mechanics* 57.4 (2016): 583-610.

Gibbs energy, mobility, σ

ICME

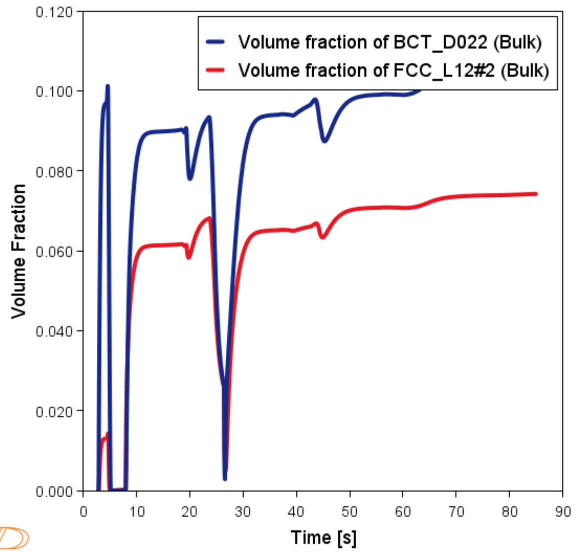
Density, C_p, ΔH

Finite Element



Thermal cycles

Thermo-Calc Software



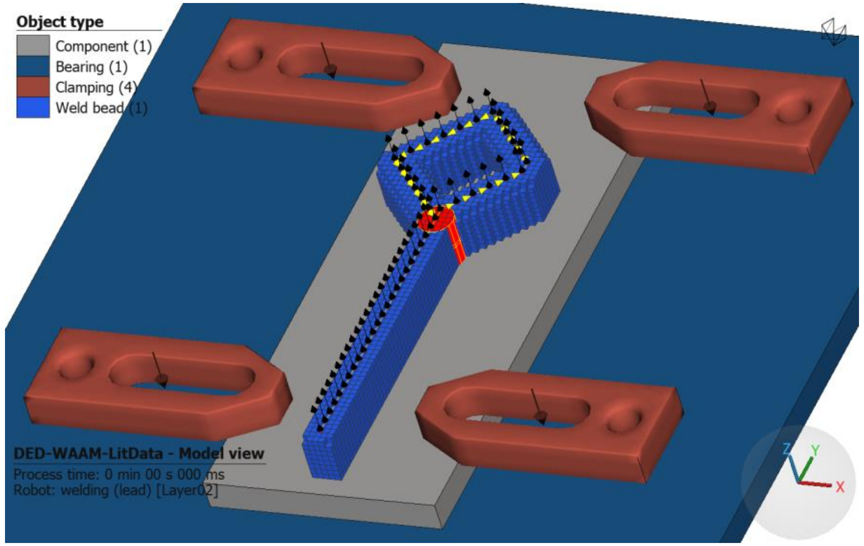
Precipitation modeling (+ mech properties?)

Kumara, Chamara, et al. *Additive Manufacturing* 25 (2019): 357-364.

This work

- Alloy 718 (simplified chemistry)
  - 316L build plate
- Thermo-Calc + TCNI11/MOBNI5 databases
  - CALPHAD + Precipitation modeling
- Simufact Welding for FEA
- One geometry
- 3 different build processes, LPBF, EBD, WAAM
- 2 input sets of data (literature and CALPHAD calculated)
  - Not all literature data is temp dependent!

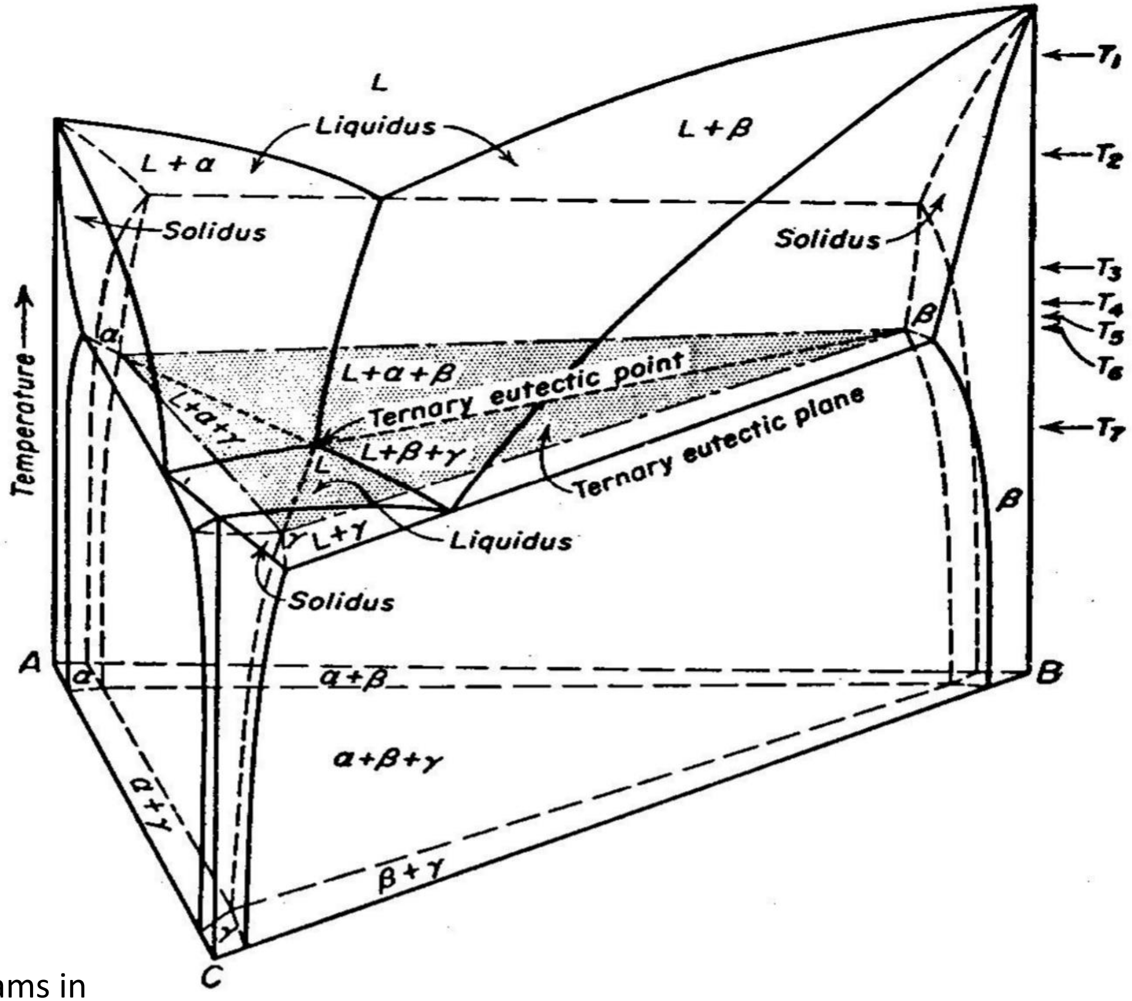
718: Ni – 17.5Cr – 19Fe – 5Nb – 3Mo – 1Ti – 0.6Al
316L: Fe – 17Cr – 12Ni – 2.5Mo – 2Mn



CALPHAD: A phase-based approach

CALculation of PHAse Diagrams

- Phase based
  - Captures composition/temperature dependence
- Binary/Ternary thermodynamic data assessed and modeled – CALPHAD database
- Self-consistent framework allows for projection into multi-component space
  - Real industrial alloys
  - Alloy design
  - Process exploration
- Binaries are the bounds of a ternary
  - Ternaries are the bounds of multi-dimensional system



F. N. Rhines, "Phase diagrams in metallurgy, McGraw-hill, 1956

CALPHAD: A phase-based approach

$$G(p,T) = H - TS$$

Gibbs Free Energy

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

Ficks Laws of Diffusion

$$\Delta G = \frac{4}{3}\pi r^3 \Delta g + 4\pi r^2 \sigma$$

Classical Nucleation Theory

(and Growth)

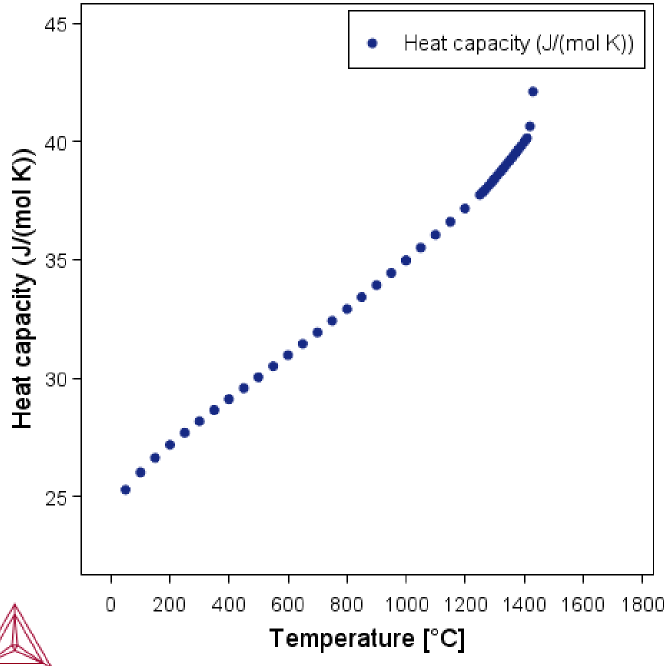
Minimize Gibbs Free Energy – Need database describing G for each phase as a function of chemistry / temp

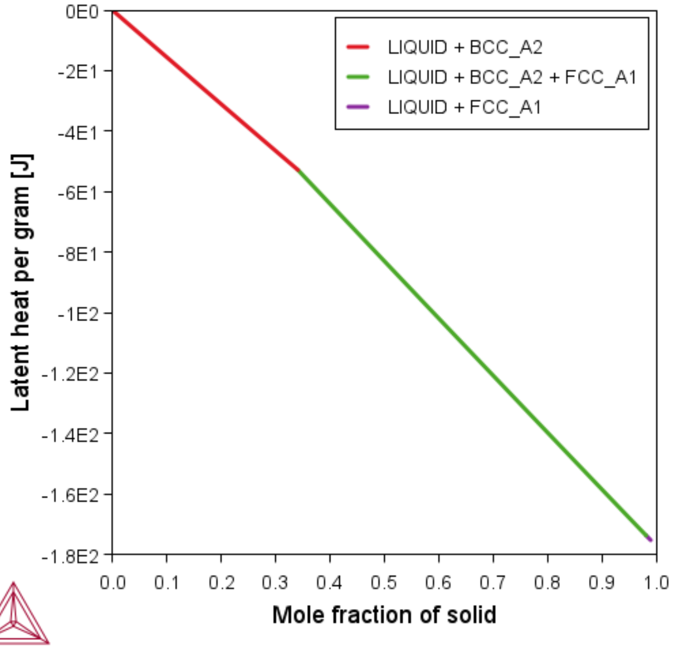
Numerically solve (FDM/FVM) – Need to describe diffusivity, done with a database of mobilities

Mean field precipitation simulation – using LS (Langer-Schwartz) and KWN (Kampmann and Wagner Numerical) Approach – Need database of σ, molar volume

Other properties:

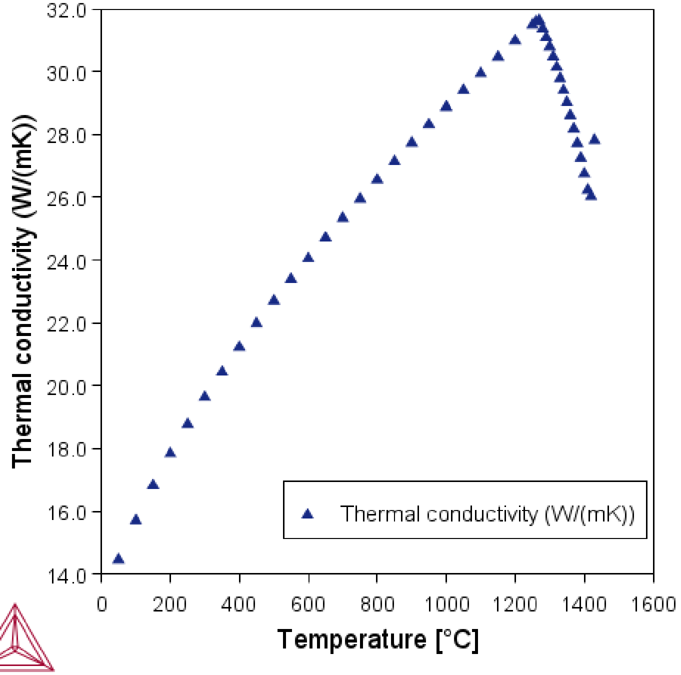
- Resistivity (electrical, thermal)
- molar volume/density
- anti-phase boundary energy
- martensite/bainite/pearlite + more

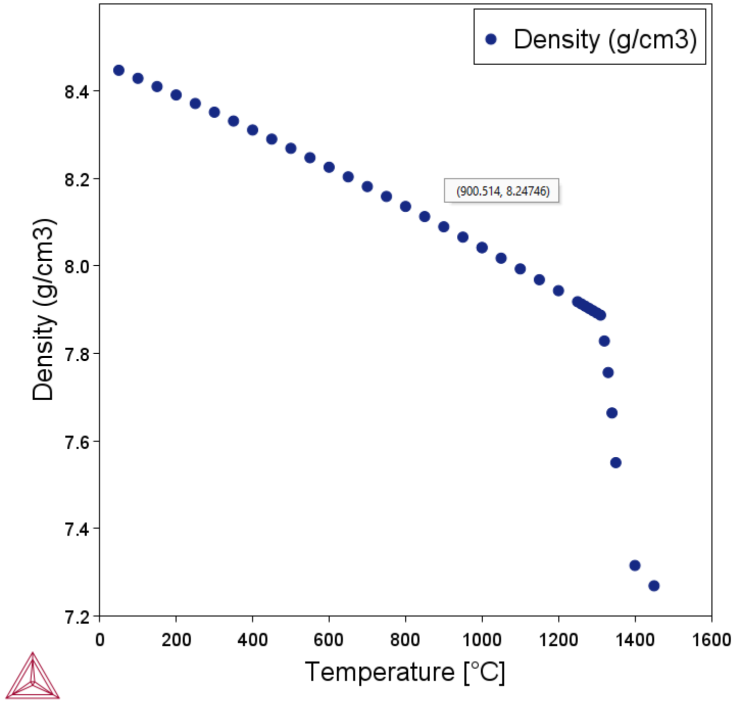




Example CALPHAD Data

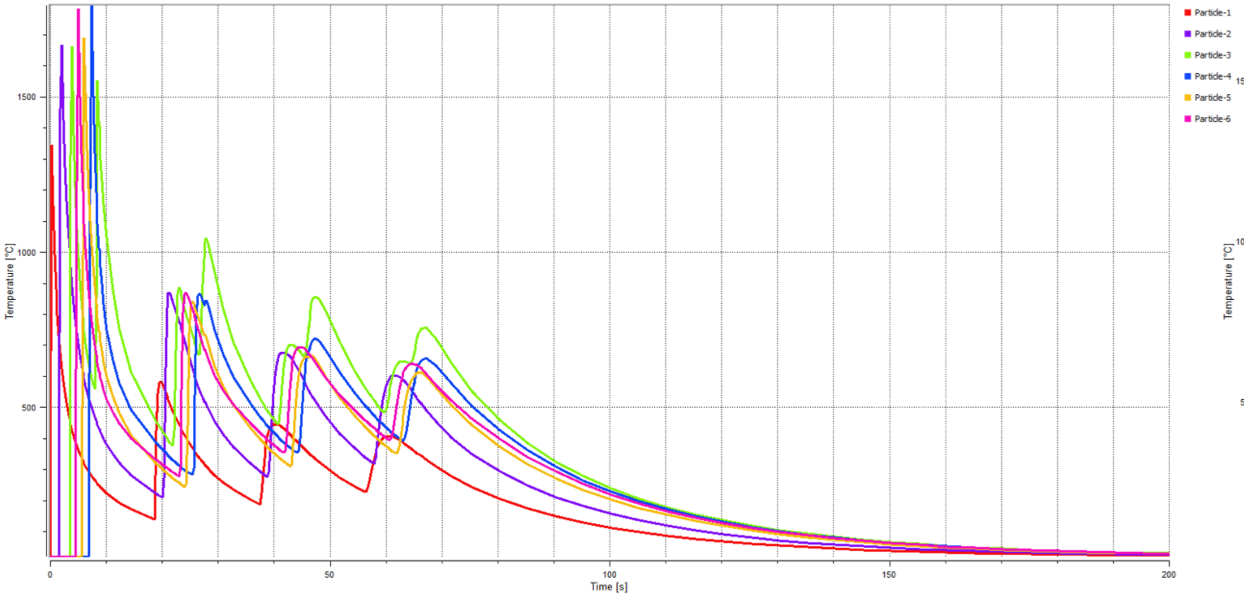
- Alloy 718
- Chemistry specific
- Function of temperature



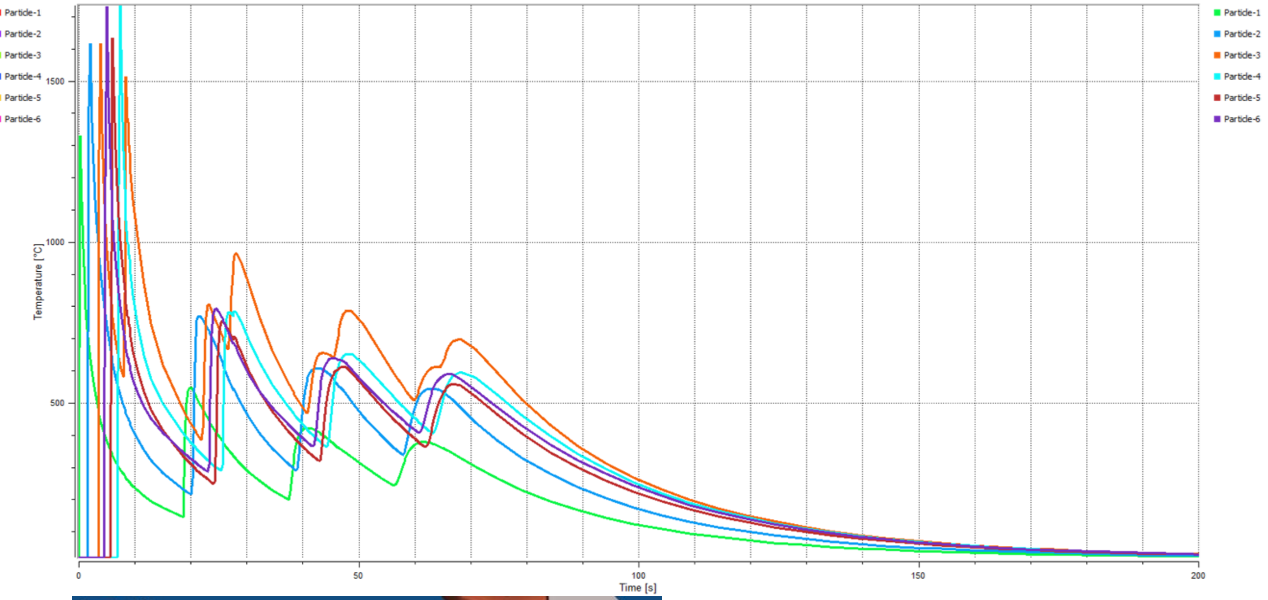


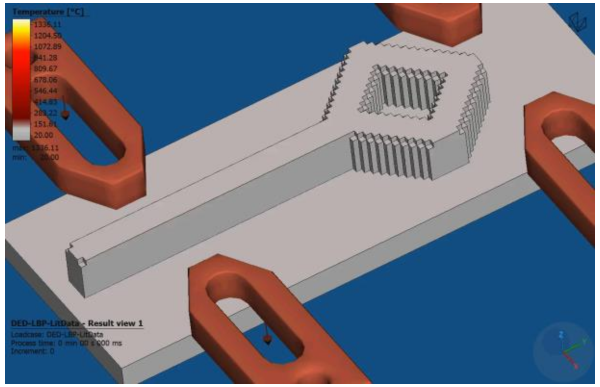
LBP Simulations

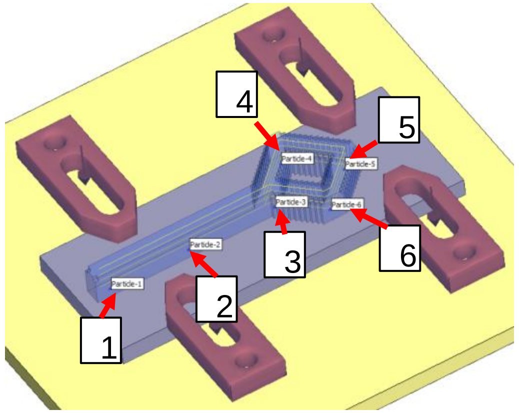
Literature Data

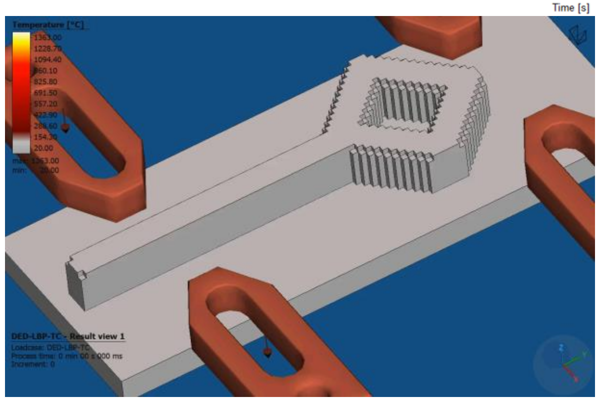


CALPHAD calculated data









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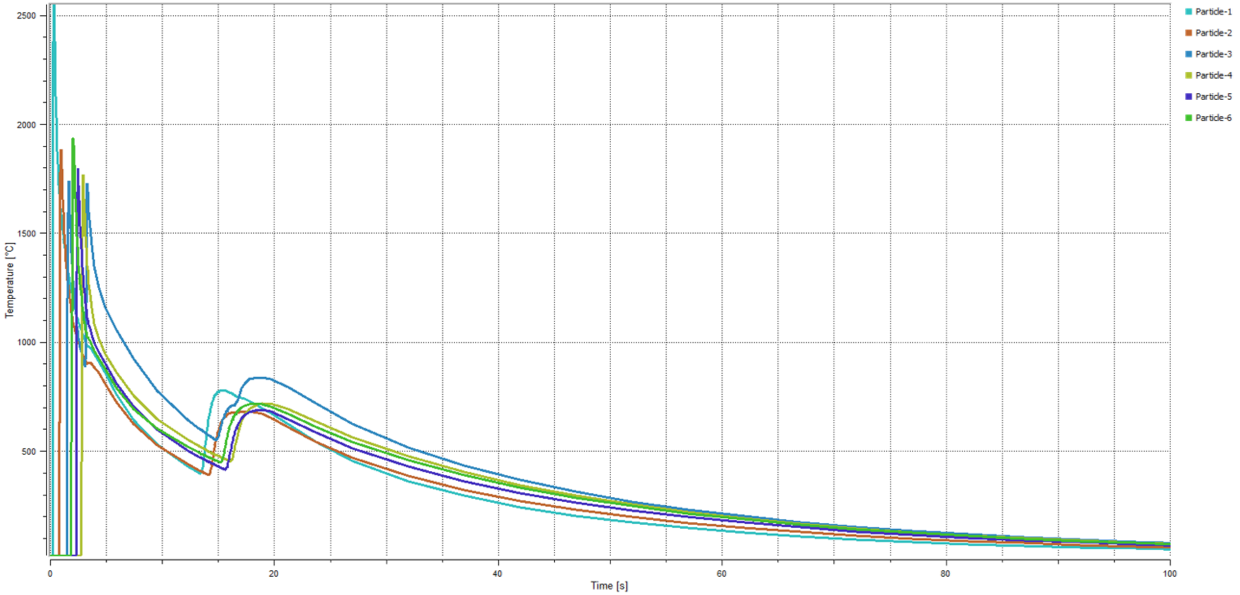
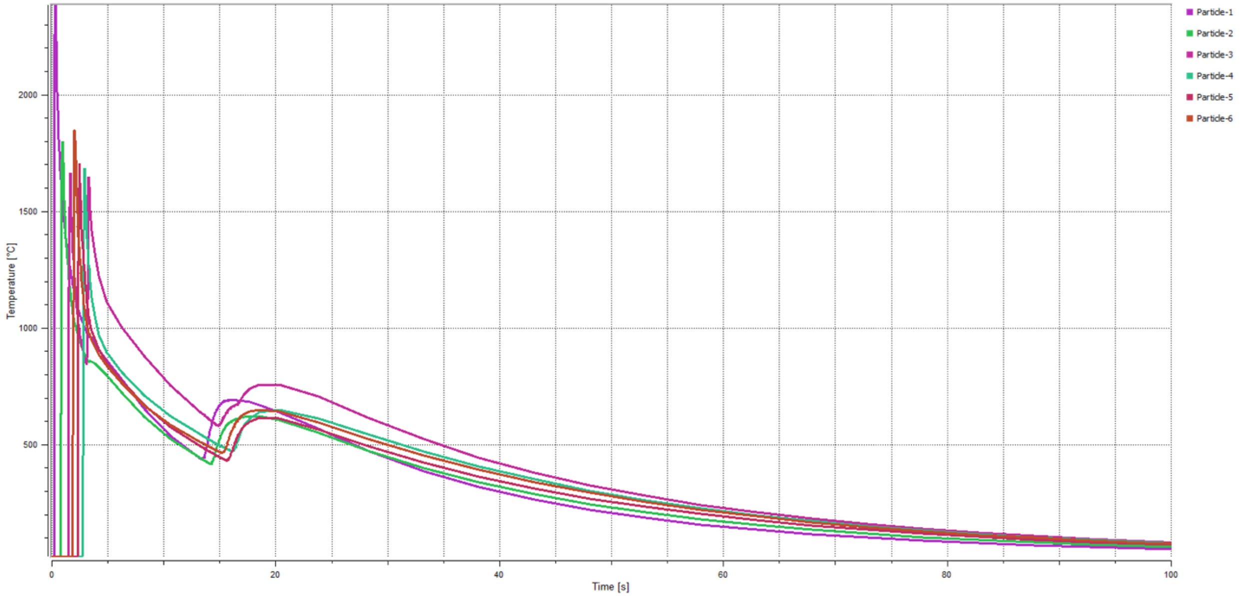
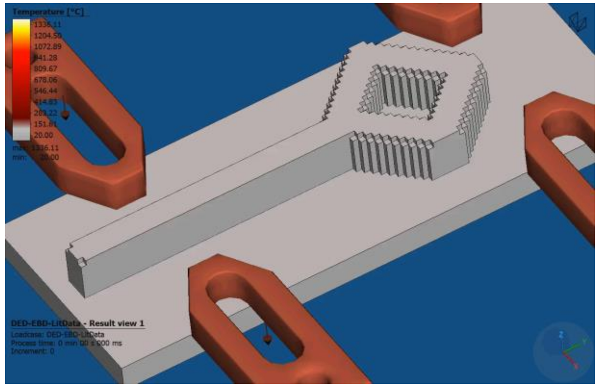
EBD Simulations

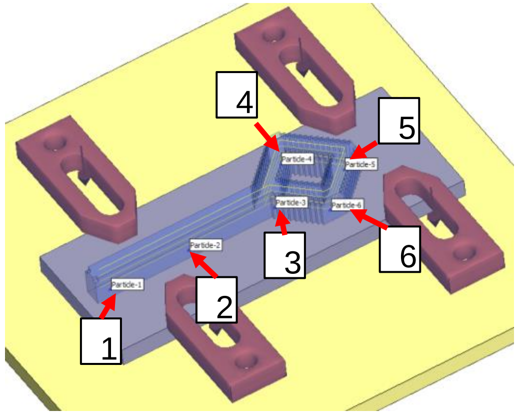
Literature Data

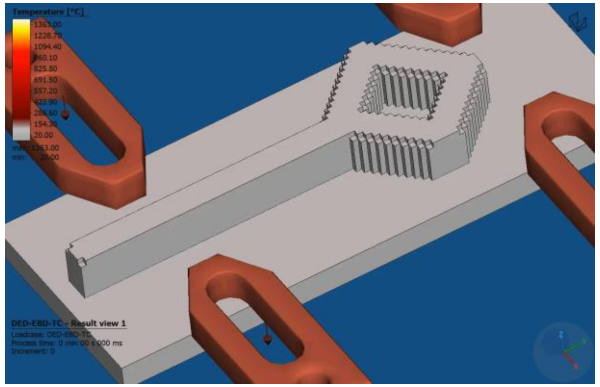


CALPHAD calculated data









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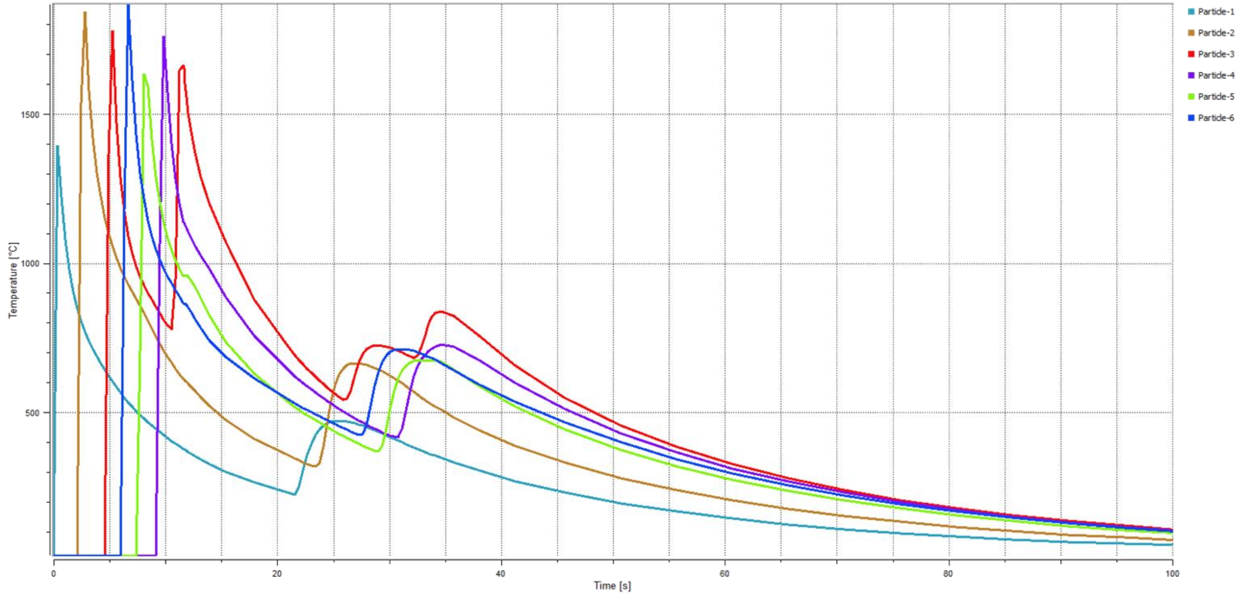
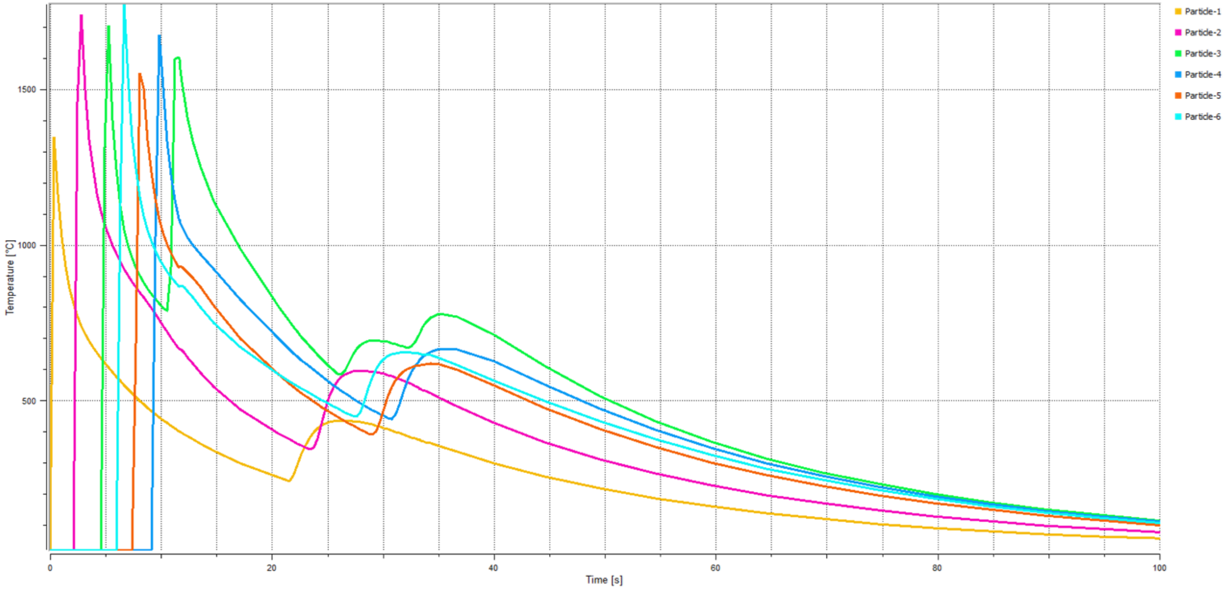
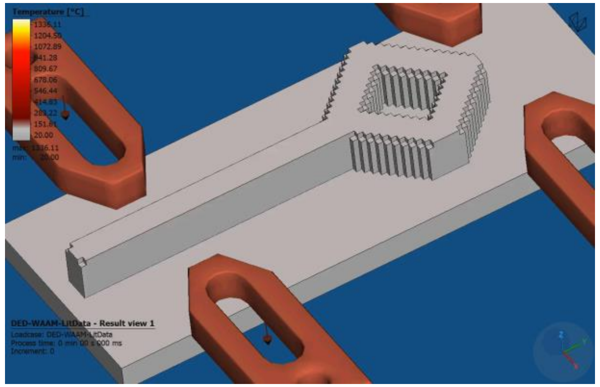
WAAM Simulations

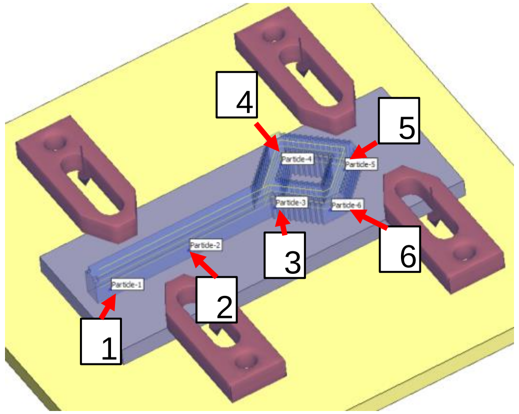
Literature Data

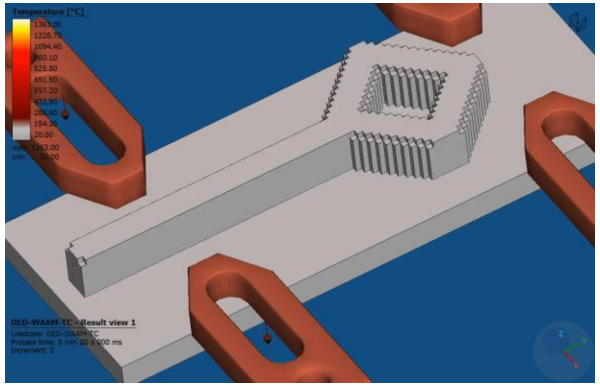


CALPHAD calculated data

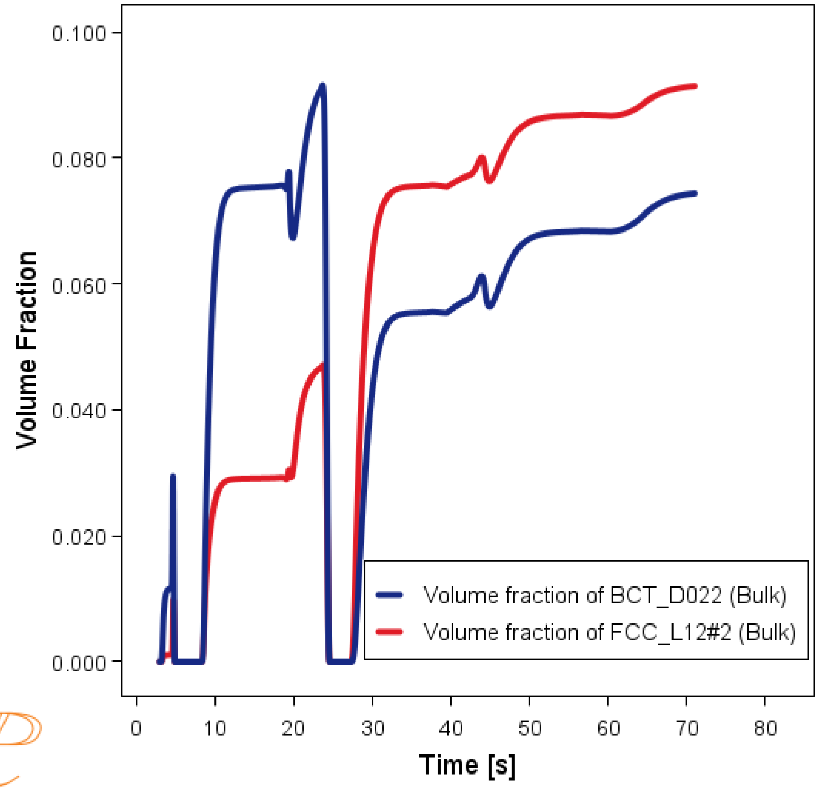


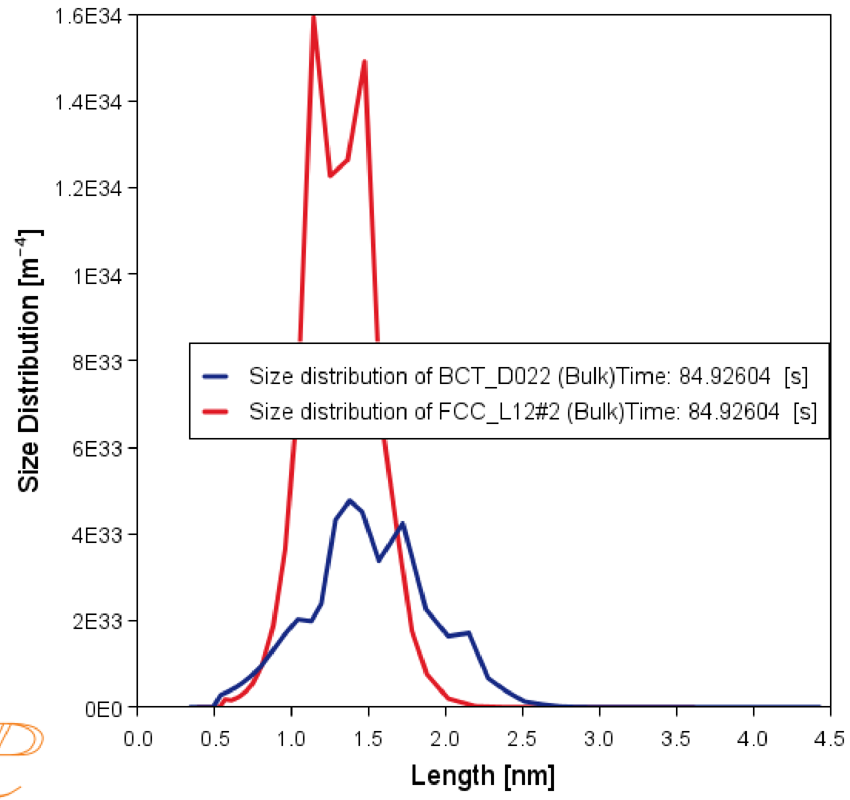




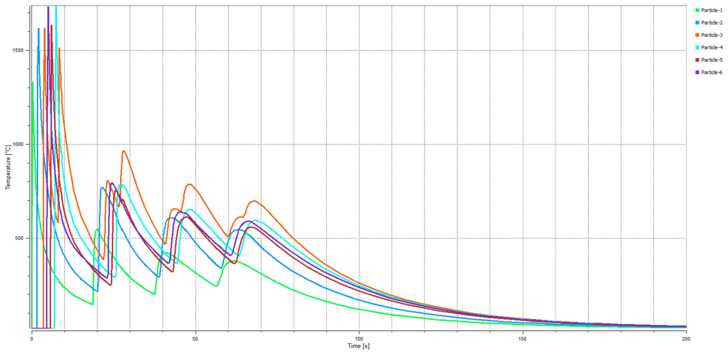


Precipitation Simulations





Point 3 – LPBF

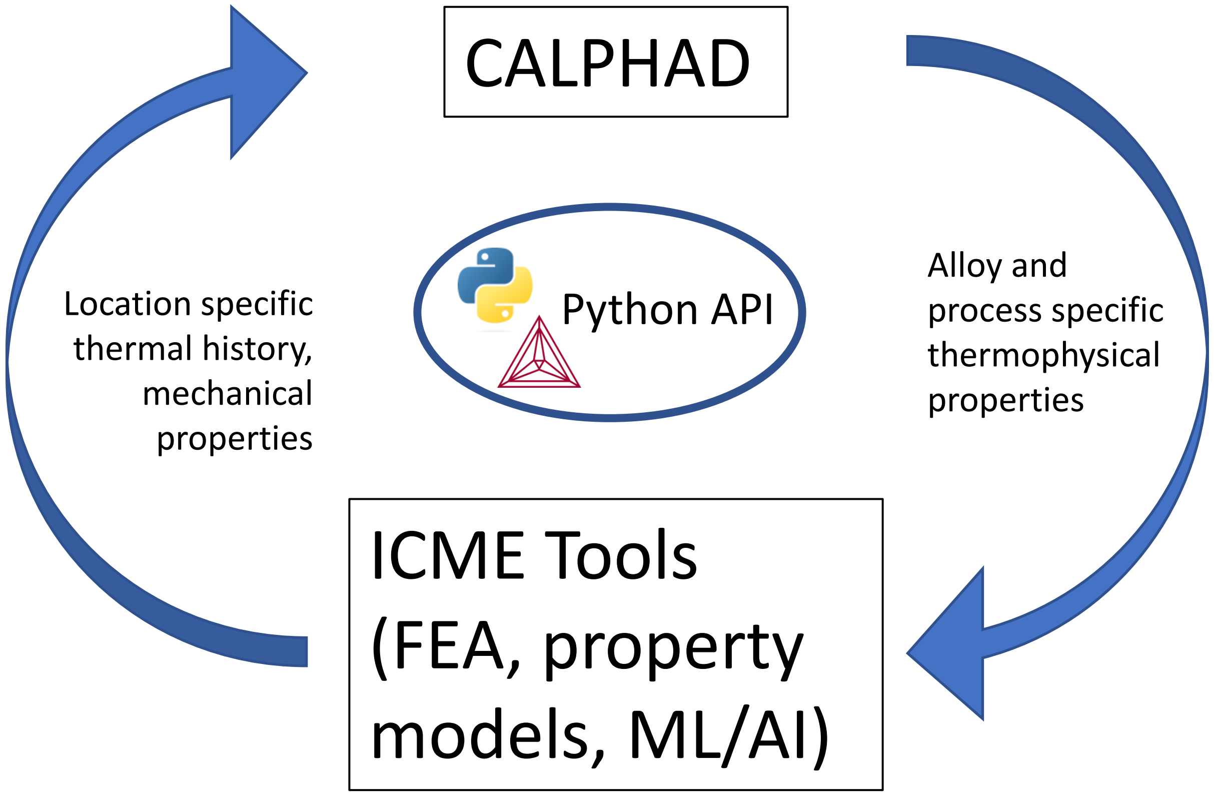


Assumptions / Future work

- Chemistries were simplified
- Segregation not taken into account
  - Laves eutectic depletes matrix of Nb, slowing precipitation
  - Chemistry gradient (core/boundary) lead to varying kinetics
    - Possible to account for this with CALPHAD
- Simplified builds
  - Could increase layers to add ‘more time’ for precipitation
- Property predictions based on precipitate distributions?

Conclusions / New Developments to improve ICME integrations

- CALPHAD based computational tools are an integral part of ICME frameworks to fill material data and knowledge gaps
- Thermodynamic and thermophysical data can be extracted and used to improve FEA type models
- Models for Thermophysical properties
  - Viscosity & surface tension (for fluid flow/combine with CFD)
  - Density for some metastable phases (for better residual stress predictions/FEM)
  - Thermal conductivity (for heat transfer/fluid flow/residual stress)
- Models for displacive transformations (martensite/bainite)
- Yield Stress
- Other models via Python (in-house, literature)



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