Materials and Solid Mechanics

LIÈGE université

Metallic Materials Science

How finite element simulations and phase field method interact to predict material properties of additive manufacturing samples

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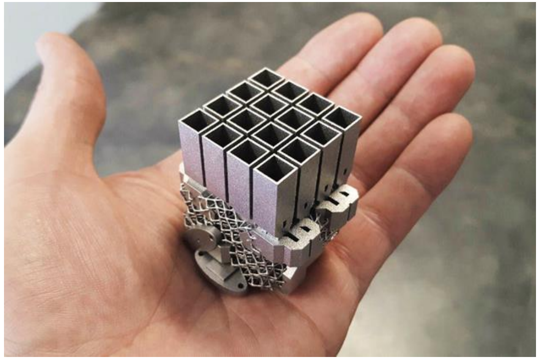
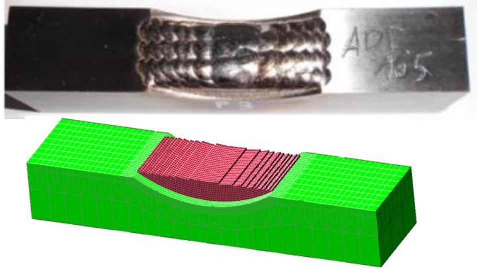
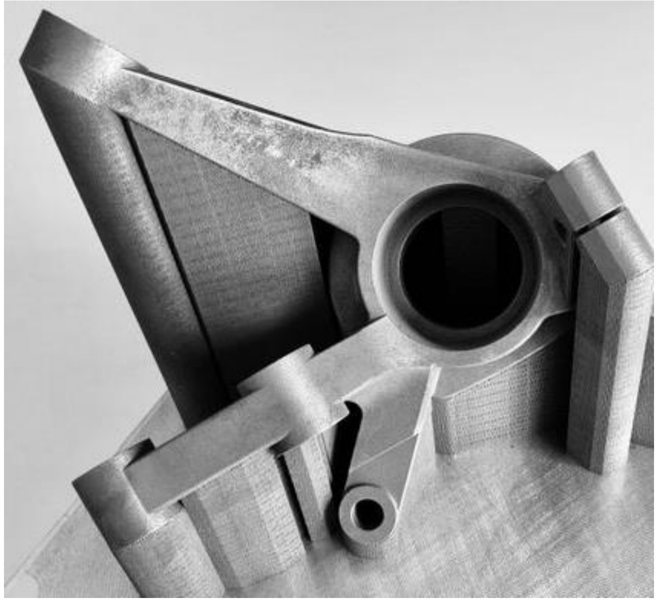
Contents







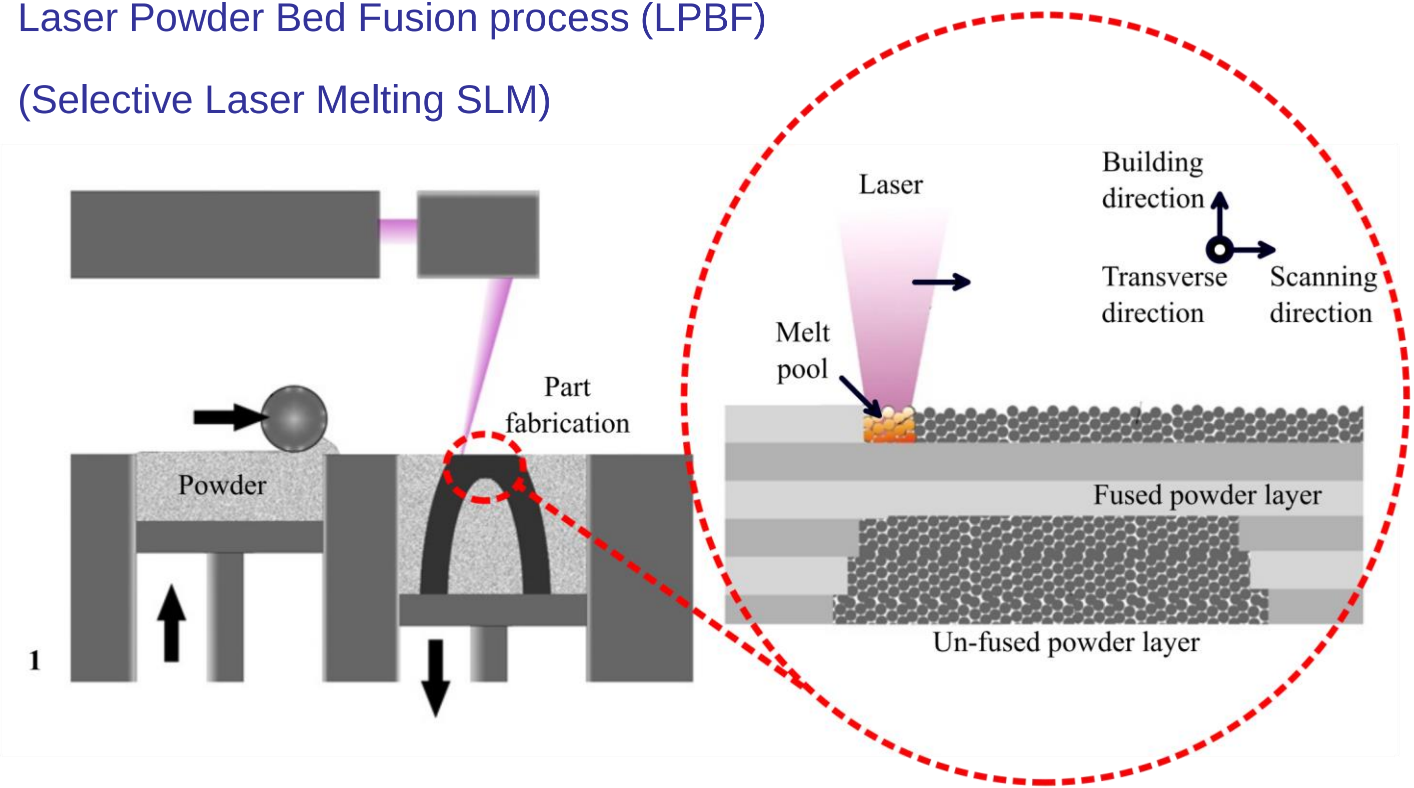
Motivation

Provide guidance in Additive Manufacturing & Post treatment

Background : the process

Laser Powder Bed Fusion process (LPBF)

(Selective Laser Melting SLM)



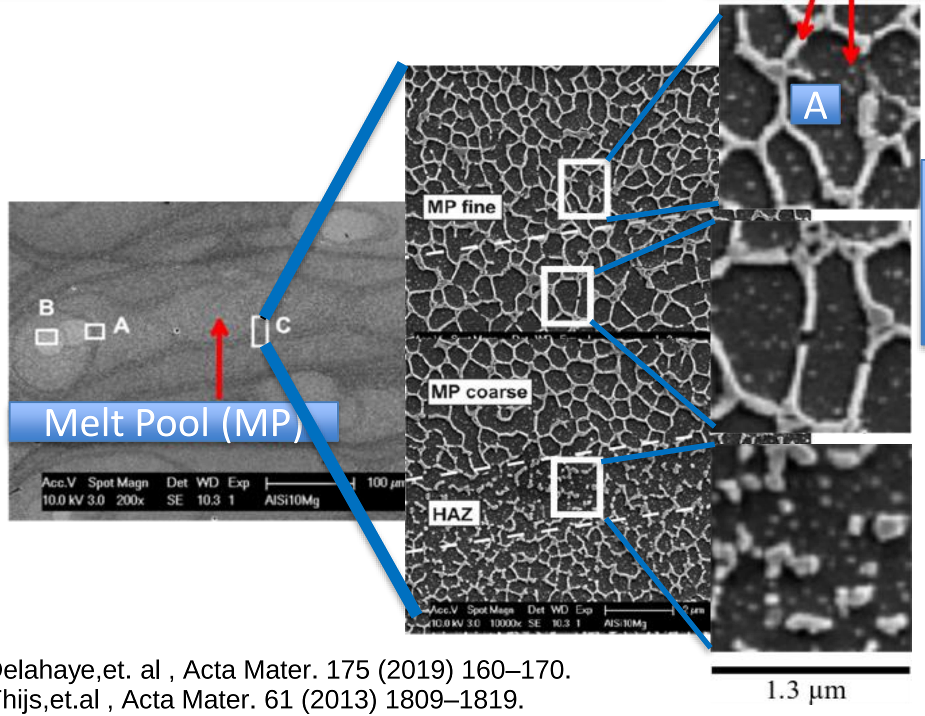
[1] https://en.wikipedia.org/wiki/Selective_laser_melting

The microstructure: bi phasic material A-B

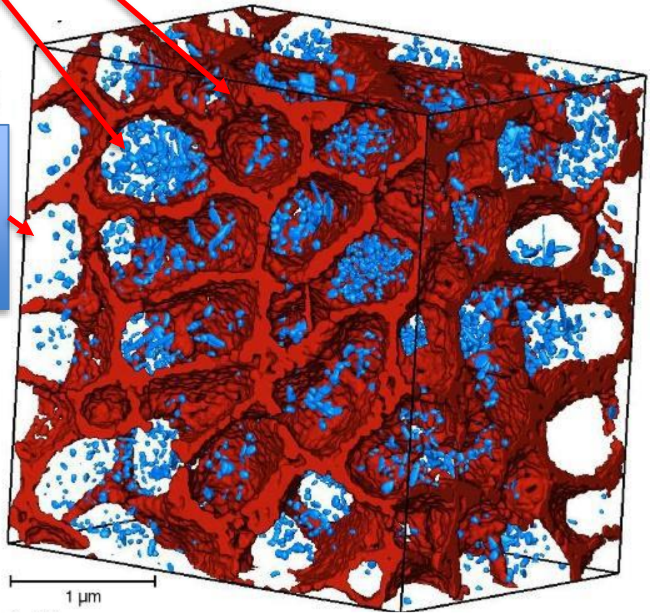
Cell Size different in the melt pool
Melt Pool core (MP Fine)
Melt Pool Boundary (MP Coarse)
Heat Affected Zone

B atoms
→ Walls (eutectic rich zone + precipitate)
→ Precipitate in the cell
→ Some in solid solution within the cell

Typical As-Built Material



A atoms
Solid
Solution



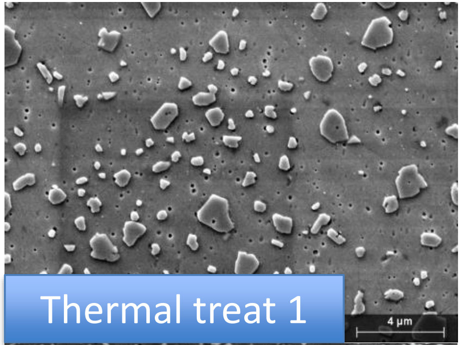
J. Delahaye,et. al , Acta Mater. 175 (2019) 160–170.
L. Thijs,et.al , Acta Mater. 61 (2013) 1809–1819.

J.G. Santos Macías et al. Acta Materialia 201 (2020)]
L. Zhao et al. Materials Science & Engineering A 764 (2019)]

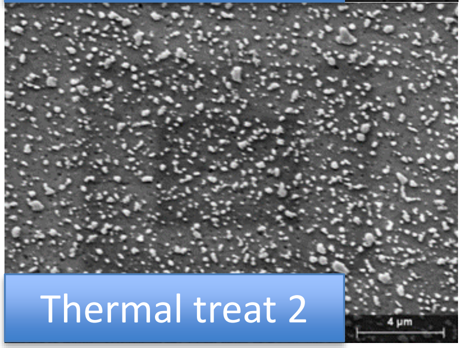
Bi phasic material evolution

Eutectic network defining wall can disappear
Globules of B material can appear
“Matrix” of A material (still solid solution)

Microstructure evolution



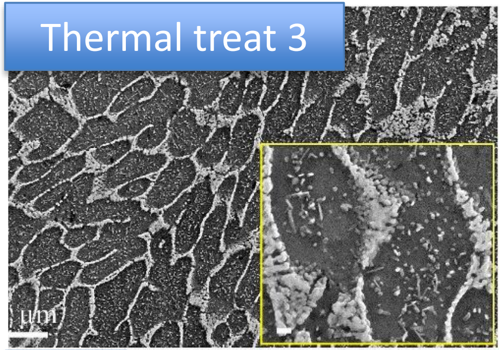
Thermal treat 1



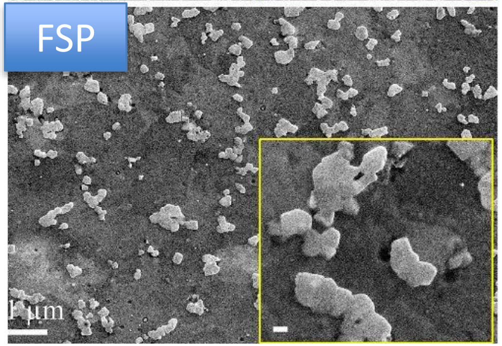
Thermal treat 2

LongLifeAM results courtesy of MMS team

Thermal treat 3



FSP

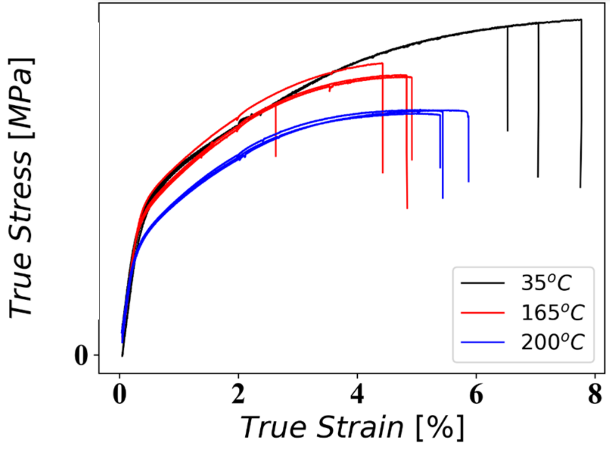


L. Zhao et al. Materials Science & Engineering A 764 (2019)]

After
Heat Treatments
Friction Stir Processing
…

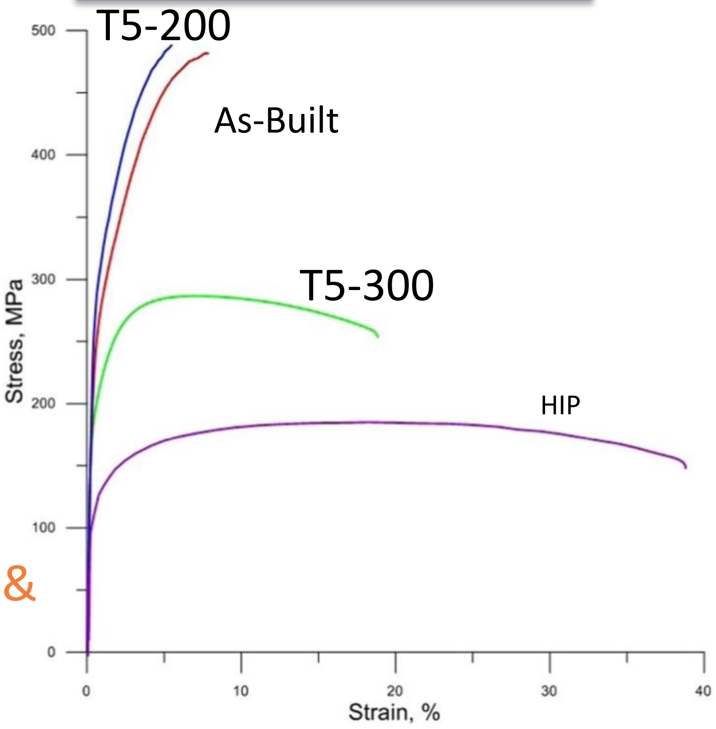
Static properties linked with microstructure

Tensile tests for different built platform tp°

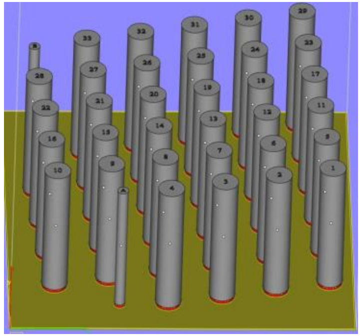


LongLifeAM results courtesy of MMS team

Tensile tests for different post treatments



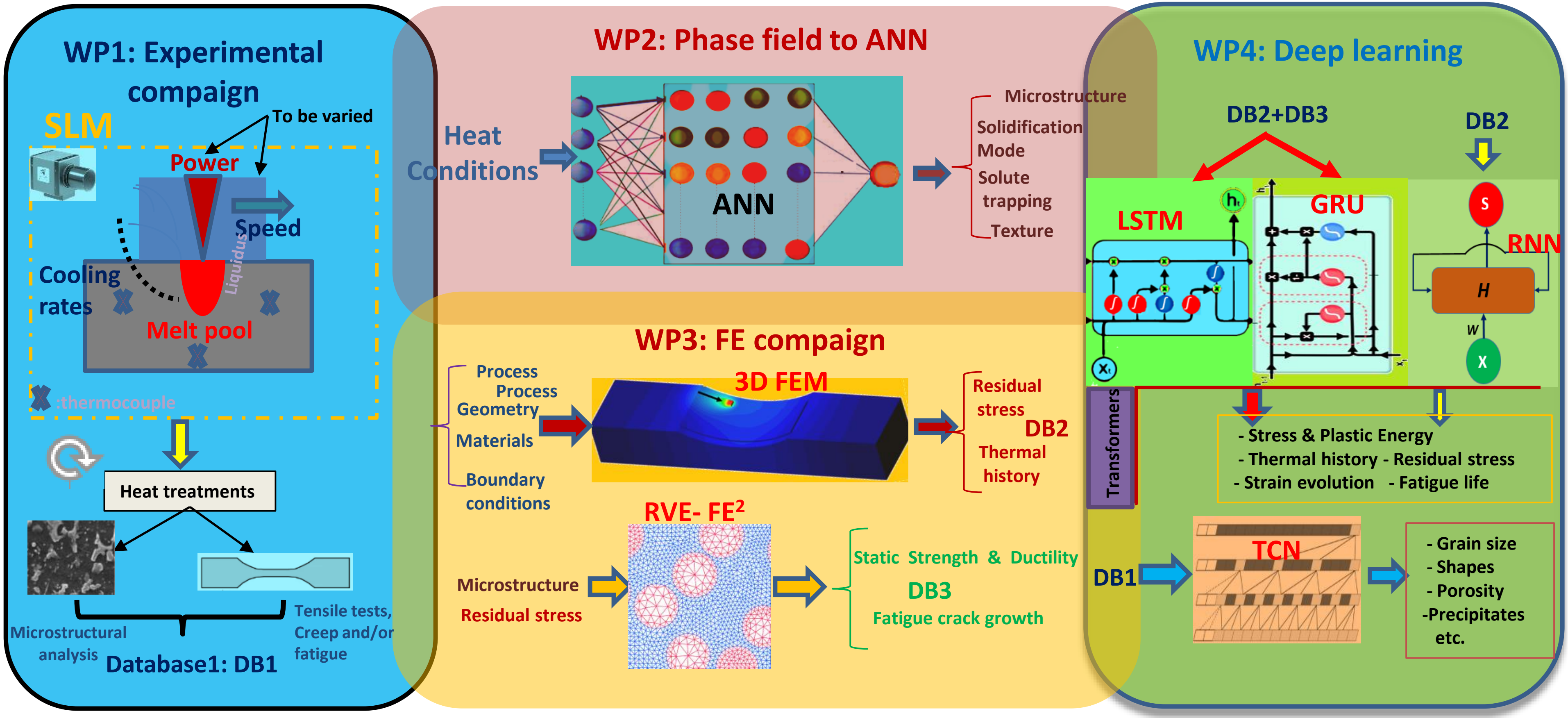
Rosenthal, et al. MSEA 729 310-22 (2018).



Selection of process parameters & post treatments could benefit some guidance

Computational Frame work

Today focus : Thermal FE and Phase Field → Microstructure



Iterative loop ?

↓

Microstructure evolution

↓

New thermo-physical properties

↓

New Temperature history

FE model

↓

Temperature history

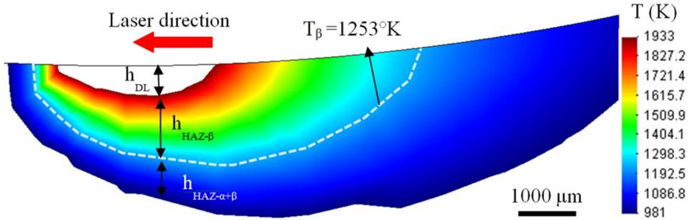
↓

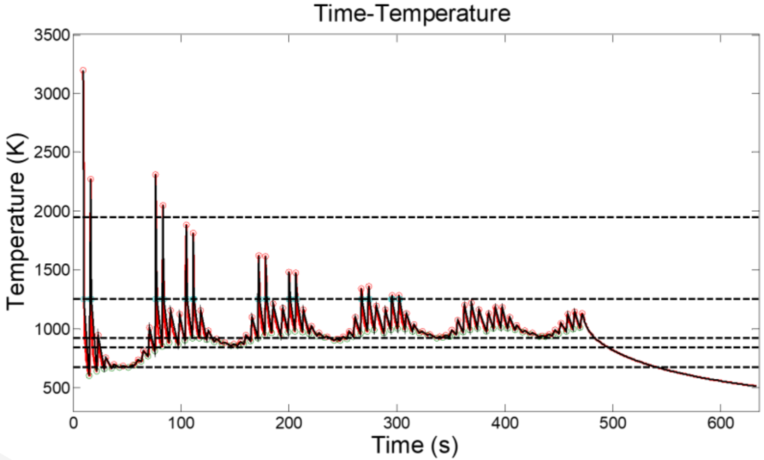
Phase Field

↓

Microstructure evolution

Final Microstructure → Final Properties



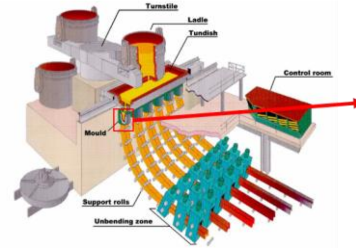


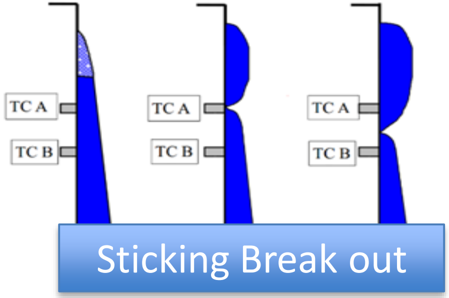
Finite Element Model

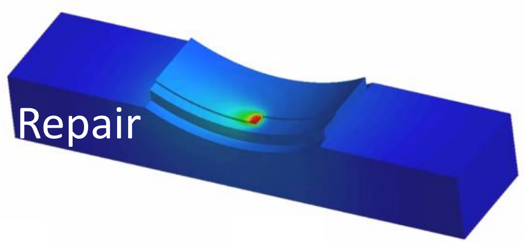
Predict the Tp° history, melt pool size…

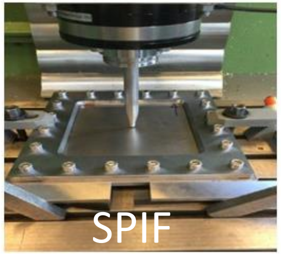
FE thermal model

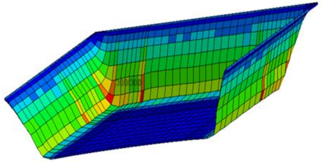
- Lagamine thermo-mechanical-metallurgical FE code (developed since 1982)





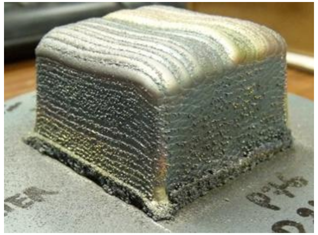






- Validated by Abaqus, Comsol, Aster **<u>and experiments</u>**
- Validated on DED for 3 materials

H.-S Tran et al. Materials & Design, 204, 128, 2017, 3D case of Ti6Al4V
R. Jardin et al. Metals 2020, 10, 1554, 3D case of M4 high speed steel
S. Fetni et al. Materials & Design, 204, 2021, 2D case of 316L + WC



- TDMU collaboration (project EDPOMP)

  → Directed Energy Deposition: FEM & Deep Learning

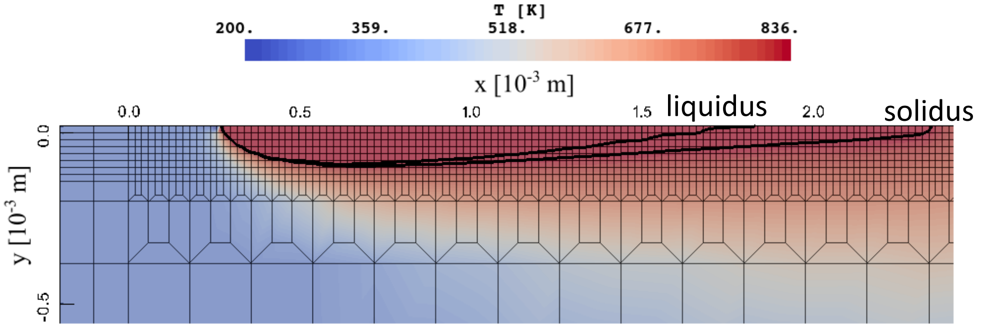
T. Quy Duc Pham et al . ESAFORM proc. 2021 **and Rice 2021**

FE thermal model applied on LPBF

- 2D model (no thermal flow in transversal direction, 1 track per layer)
- Birth element technique
- Solid model (no fluid movement, just by increased conductivity)
- **Laser absorptivity**, convection and radiation coefficients adjusted to recover: melt pool size & cell size
- Material data: Heat capacity c_p and conduction k
- Mesh convergence studied

→ Temperature history for each material point

→ Melt pool depth and width



Thermal finite elements model of LPBF

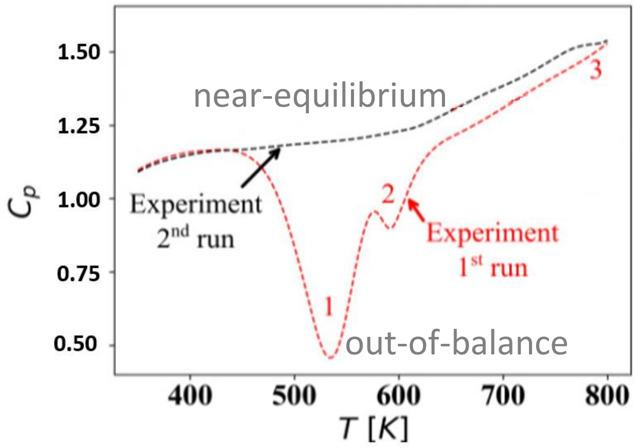
[PhD Delahaye unpublished results 21]

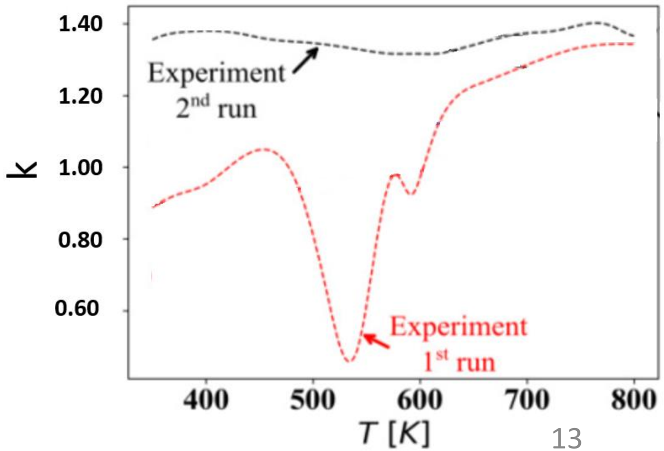
Input Material data

- c_p and conduction k measured on LBFP samples
- **BUT** differential scanning calorimetry (DSC) measurement = bad ‘twin’

Cooling / heating rate: 10^6 K.s^{-1} for LPBF ≠ 1.7 K.s^{-1} for DSC

1. B atoms from sur saturated solution diffuse to B precipitates
2. B precipitates growth
3. Walls dissolve





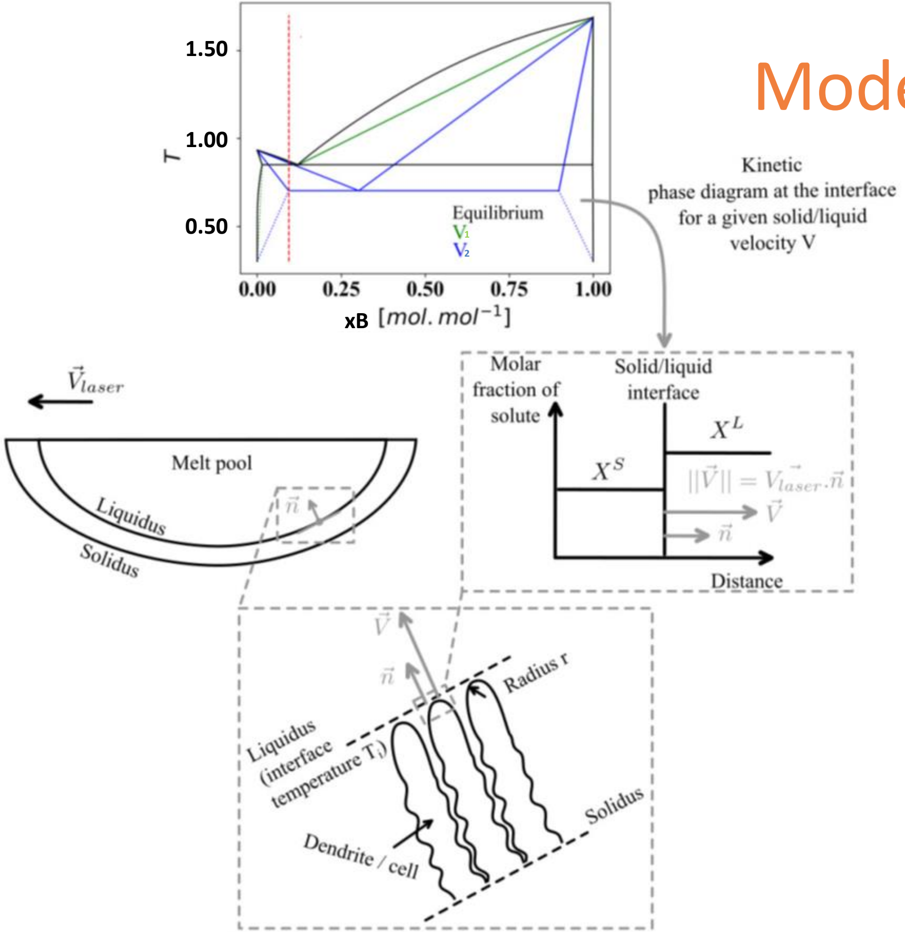
Model improvement?

Instantaneus c_p and k computed on real temperature history

4 Different models

1. Calphad approach (A-B equilibrium phase diagram)
2. Calphad apparent (Diagram shifted: heat absorbed by dissolution of ‘wall’)
3. New implemented model with kinetic effect of liquid solid interface & Sur saturation due to the high cooling rate in LPBF
4. Post processing of microstructure result of Phase Field simulation

Model 3: Conductivity model



-microstructure AB in equilibrium

-microstructure AB out of balance (sur saturation of B in A solid solution)

→ Dendrite growth model under non equilibrium conditions

→ no diffusion in solid

→ Infinite diffusion in liquid

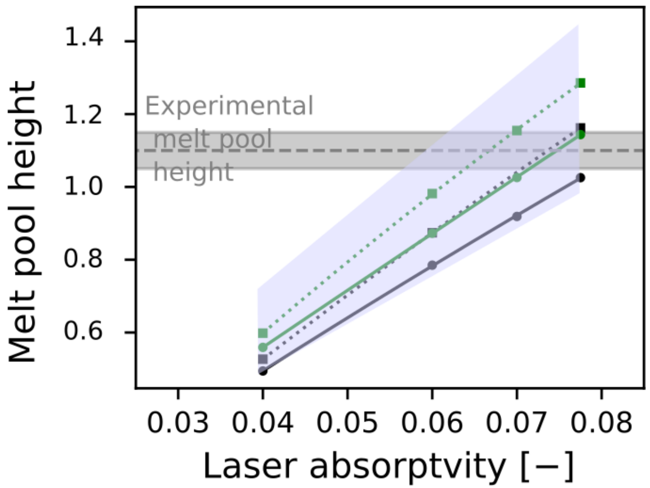
R. Trivedi and W. Kurz, Dendritic growth, International Materials Reviews 341 39 (2) (1994)

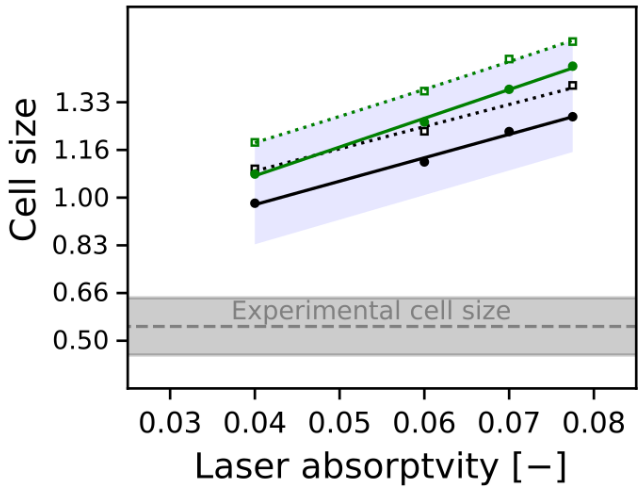
w. J. BOETTINGER, S. R. CORIELL, and R. TRIVEDI: 'Fourth conf. on rapid solidification 13; 1988, Baton Rouge, LA, Claitor's Publishing Division.

FE simulation sensitivity

For fixed convection & radiation coefficient,
Identified laser absorptivity highly depends on input data

FE Prediction





FE Assumptions

c_p and k

Shaded zone:
Calphad or new

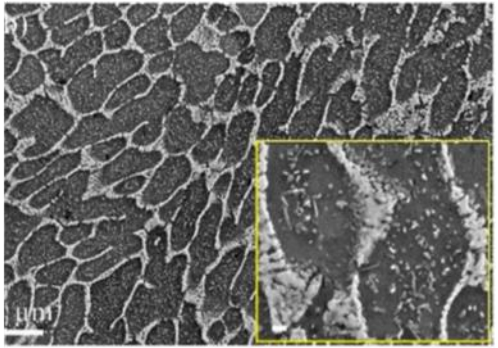
DSC experiment

— 1st Run
— 2nd Run

… Marangoni
k x 2

Why ? 2D FE assumption + *Marangoni* not accurate

(*liquid convection generated by variable surface tension in the melt pool*)



As built

After post processing

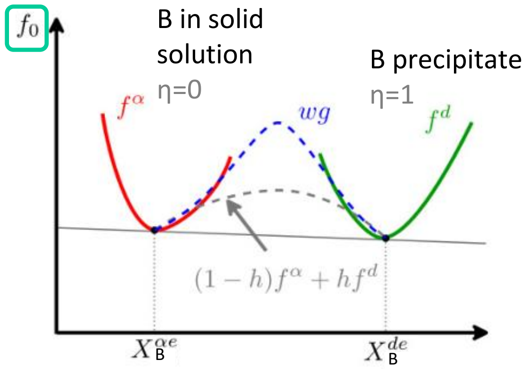
Phase Field Model

Predict microstructure evolution

Phase Field Model description (1/4)

Free energy formulation

- Kim Kim Suzuki model to compute the phase η
- Interface considered as mixture of both phases A and B with the same chemical potential



Non-homogeneous free energy

Homogeneous free energy density

$$\mathcal{F} = \langle V_m \rangle \int_V f_0(X_B, \eta, T) + \frac{\kappa^2}{2}(\nabla\eta)^2 + e_{el}\, dV$$

Average molar volume

Molar fraction of B in A

Phase

Temperature

Interface contribution

Elastic strain energy

$$f_0(X_B, \eta, T) = \frac{1}{\langle V_m \rangle}[(1 - h(\eta))f^\alpha(X_B, T) + h(\eta) f^d(X_B, T) + wg(\eta)]$$

Interpolation function

Double-well potential function of height w

S.G. Kim, W.T. Kim, T. Suzuki, (1999) 12.
J.Z. Zhu, T. Wang, A.J. Ardell, S.H. Zhou, Z.K. Liu, L.Q. Chen, Acta Materialia 52 (2004) 2837–2845.

Phase Field Model description (2/4)

Elastic strain energy

$$\begin{cases} \nabla_j \sigma_{ij} = 0 \\ \sigma_{ij} = C_{ijkl}(\epsilon_{kl} - \epsilon^0_{kl}) \end{cases}$$

Stresses

Total strain

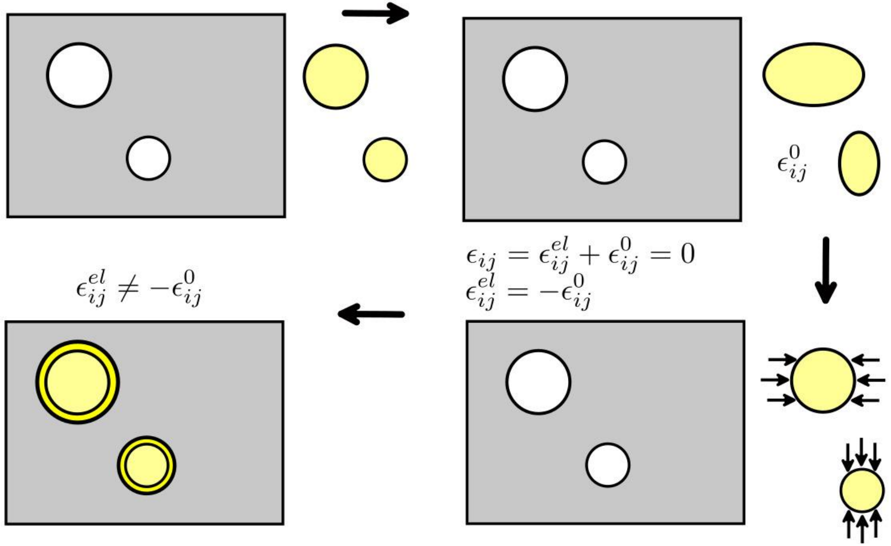
Eigen strain

Elastic strain

Stiffness tensor

$$e_{el} = \frac{1}{2} C_{ijkl}(\varepsilon_{ij} - \varepsilon^0_{ij})(\varepsilon_{kl} - \varepsilon^0_{kl})$$

A. Khachaturyan, Theroy of Structural Transformations in Solids, 1983.



Phase Field Model description (3/4)

Enhanced diffusion by quenched-in vacancies

Modified impurity diffusion coefficient of B in A

Original impurity diffusion coefficient of B in A

$$ {}^*D_B^A = \left(\frac{X_{Va}}{X^e_{Va}}\right) {}^*D_{0B}^A exp\left(-\frac{Q_{{}^*D_B^A}}{RT}\right) $$

Molar fraction of B in A matrix

$$ D_{Va} = \frac{X_{Va}}{X^e_{Va}}(X_B\, {}^*D_B^A + (1 - X_B)\, {}^*D_A^A) $$

Non-equilibrium vacancy site fraction

Vacancy diffusion coefficient

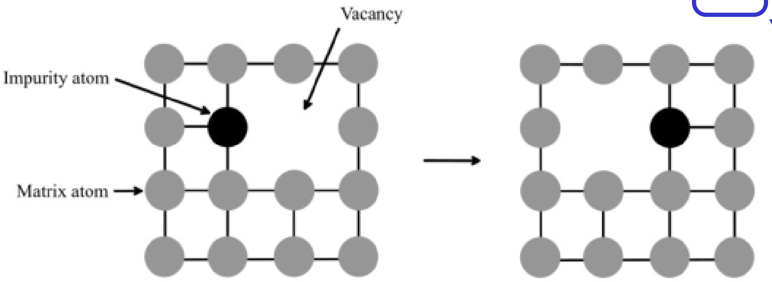
Temperature (time)

Self-diffusion coefficient of Al

$$ X_{Va}(t+dt) = X_{Va}(t) + \left[1 - exp\left(-\frac{D_{Va}}{L_{Va}^2}dt\right)\right][X^e_{Va}(T(t)) - X_{Va}(t)] $$

Vacancy site fraction at equilibrium

Mean vacancy diffusion path



A. Falahati, et al. , IJMR 101 (2010) 1089–1096.

Phase Field Model description (4/4)

Governing equations

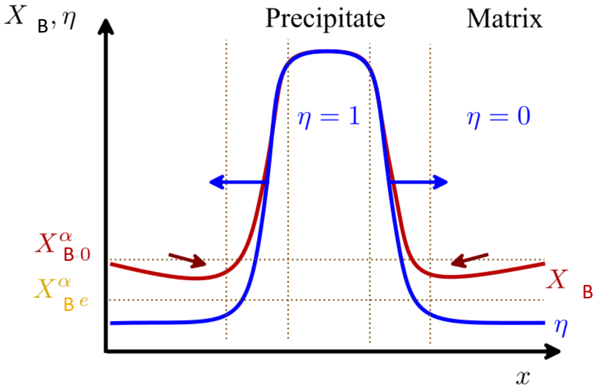
- Cahn-Hilliard for conserved field (A and B quantity)
- Allen-Cahn for non-conserved field (phase η)
- Solved by Fourier spectral methods

A/B Inter-diffusivity

$$\frac{\partial X_B}{\partial t} = \nabla . \left(\frac{\boxed{\tilde{D}}}{\partial^2 f_0 / \partial X_B^2} \nabla \frac{\delta \mathcal{F}}{\delta X_B} \right)$$

Interface kinetic coefficient

$$\frac{\partial \eta}{\partial t} = -\boxed{L} \frac{\delta \mathcal{F}}{\delta \eta}$$



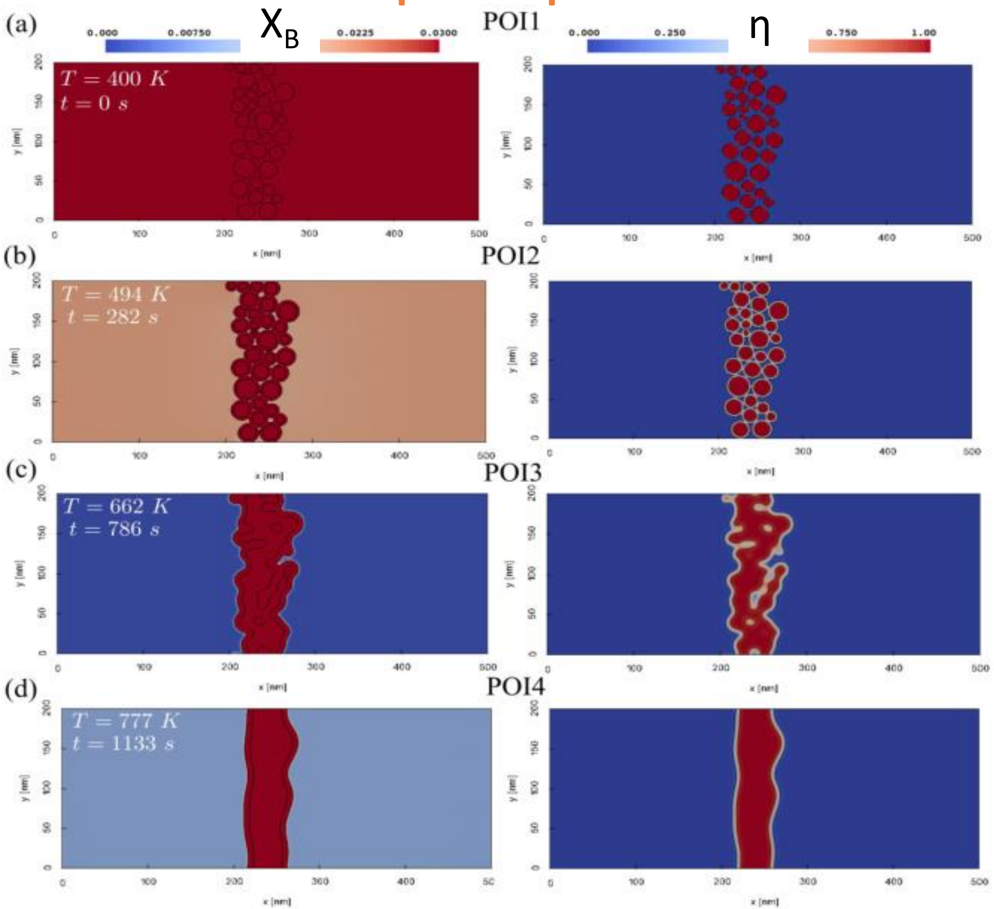
J. Zhu, L.-Q. Chen, J. Shen, V. Tikare, Physical Review E 60 (1999) 3564–3572.

Phase Field Model input

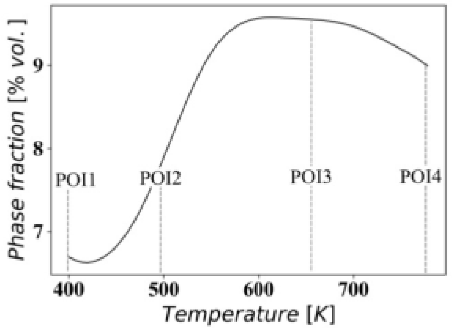
Model parameter	Symbol	Simplification	Tool / experiment	Reference
Free energy density	f^{α}, f^{d}	Parabola fitting	CALPHAD modeling	[ANS98]
A/B Inter-diffusivity	$\tilde{D}$	A/B Impurity diffusion coefficient		[Man+09]
A Self-diffusivity	$^{*}D_{A}^{A}$			[Man+09]
Interfacial mobility	M_{η}		DSC experiment	No published yet
A/B interface energy	γ		Back calculation from nucleation rate experiment	[ROS58]
Initial conditions (phase fraction and molar fraction of B)	η^{0}, X_{B}^{0}		XRD + SEM analysis	No published yet
Molar volume	V_{m}		CALPHAD modeling	[Hal07]
Stiffness tensor	C_{ijkl}	Use A value for the whole system	CALPHAD modeling	[Su+15]
Equilibrium vacancy site fraction	X_{Va}^{e}			[Meh07]

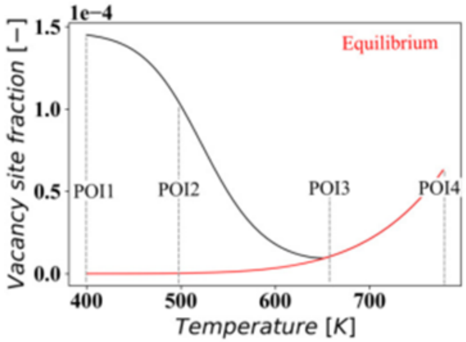
Ansara,et al. , COST 507 - Definition of Thermochemical and Thermophysical Properties to Provide a Database for the Development of New Light Alloys, 1998. Mehrer, Diffusion in Solids: Fundamentals, Methods, Materials, Diffusion-Controlled Processes, Springer Science & Business Media, 2007. Rosenbaum, D. Turnbull, Acta Metallurgica 6 (1958) 653–659. D. Su, et al. ICISMME, 2015. Hallstedt, Calphad 31 (2007) 292–302.
Mantina,et al. , Acta Materialia 57 (2009) 4102–4108

Phase Field simulation of a rich eutectic zone with B precipitates within a matrix A



for a heating rate of 20 K/min



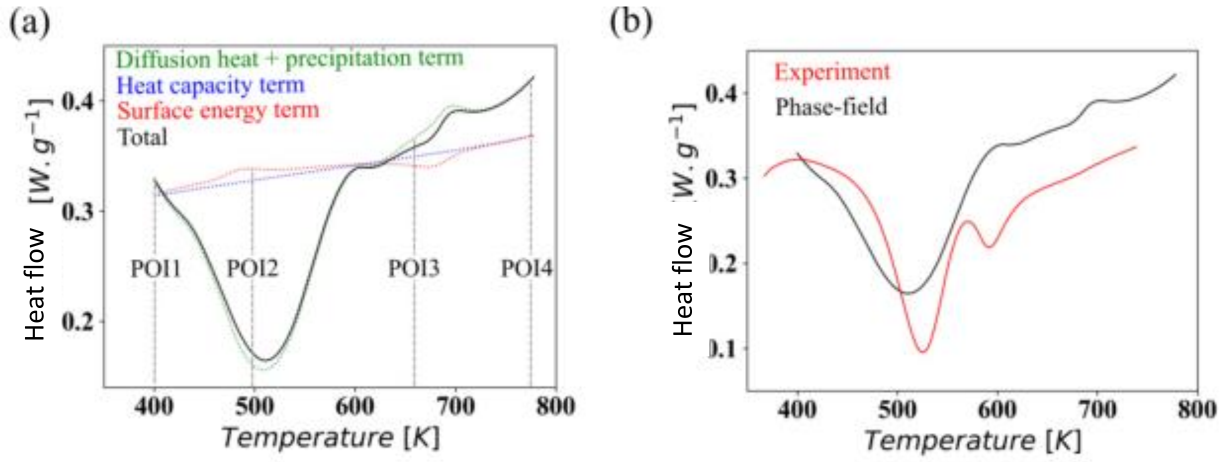


Validation on experimental DSC curve

- Frist peak (desaturation of A matrix with B) well simulated
- Second peak (B precipitate coarsening) shifted to high temperature

  → need to tune model input parameters

→ 4th model for predicting DSC and deriving c_p and k



Conclusion

On the way

- FE improvement (Marangony and 3D) : 2D FE partially validated
- Phase Field simulations (time step) → microstructure for LPBF:
  Computations validated on DSC

→ Data Bases

→ Deep Learning ↘ CPU

→ Process and post process optimization to reach ideal microstructure

- Final Microstructure → Final properties
  HAZ thickness explains fracture strains

J. Delahaye, et al. , Acta Mater. 175 (2019) 160–170

Thank you for your attention

Questions ?

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