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Wire Arc Additive Manufacturing of Advanced Steam Cycle Components Using Location Specific Design Enhanced by High-Throughput Experiments and Machine Learning

PMMD

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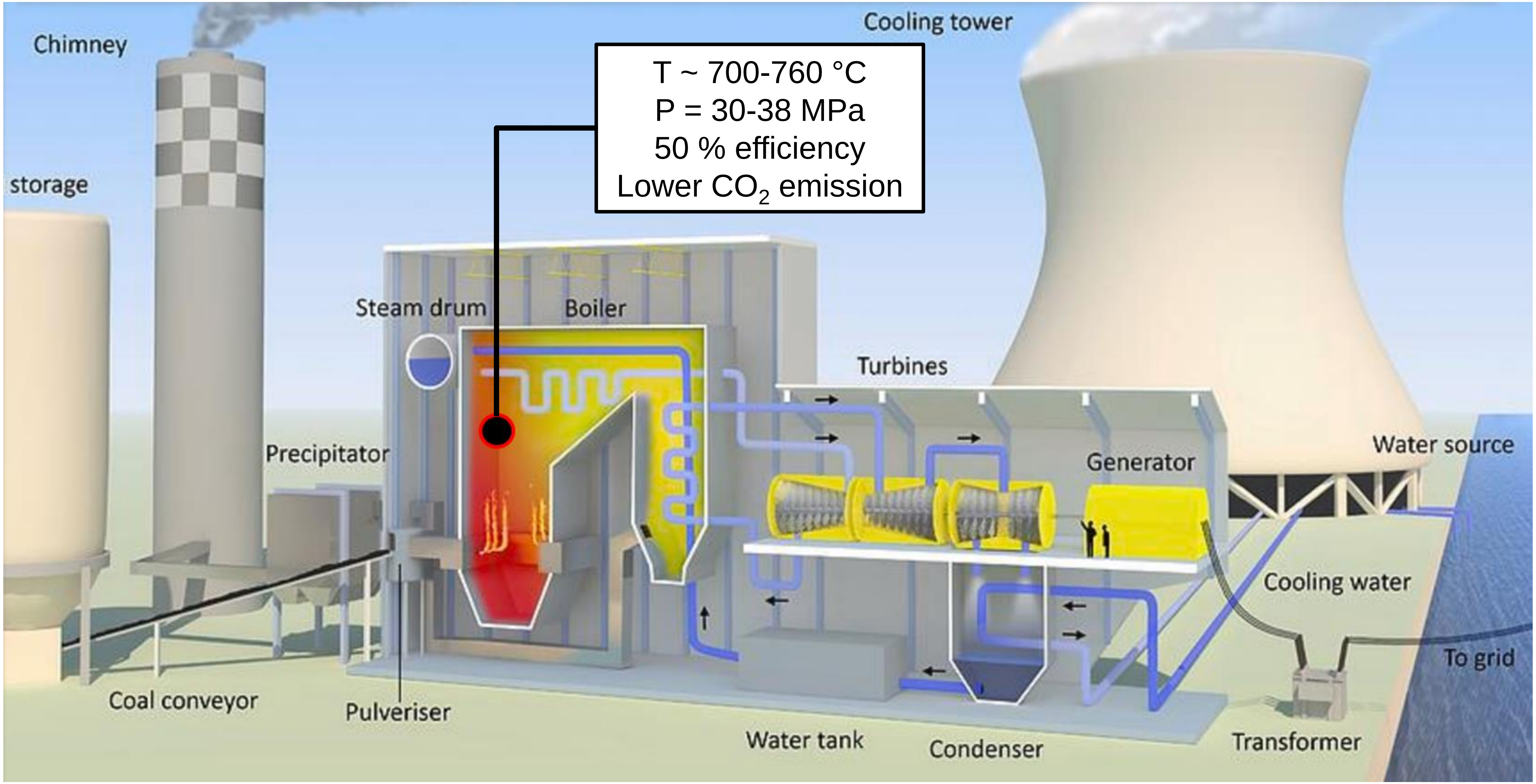
NATIONAL ENERGY TECHNOLOGY LABORATORY | PennState | SIEMENS energy | GEFERTEC | HAYNES International | University of Pittsburgh

Motivation: A-USC Coal Power Plants Eco-Efficiency



Wire Arc Additive Manufacturing (WAAM)

Challenges in WAAM of Complex Shape Thick Wall Components

(1) Distortion (3) Detrimental phase formation **(6) Location specific structure optimization**
(2) Cracking (liquation and residual stress) (4) Grain refinement (5) Precipitation strengthening

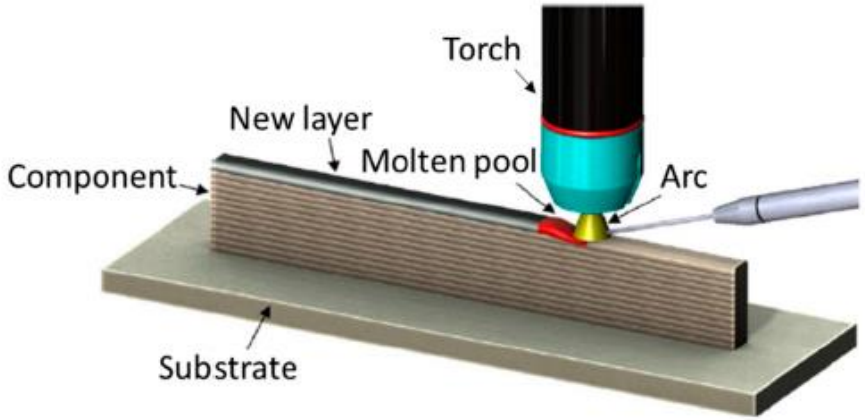
WAAM process | Post-heat treatment

Design Solutions using the Extended ICME Platform at Pitt

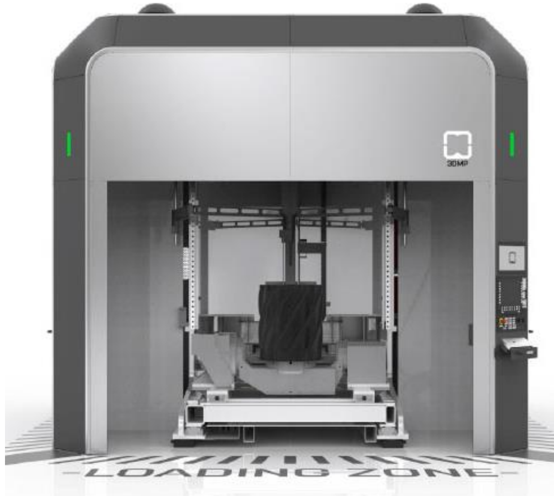
(1,2,4,6) ML-enhanced residual stress simulation (3,4,5,6) **High-throughput experiments**
(1,2) Thermodynamics informed melting (6) **Machine learning (ML) of PSP relationships**
(2,3,4,5) CALPHAD-based Phase transformation modeling (2,3,6) Grain texture simulation

Technical Collaboration HAYNES International | NETL National Energy Technology Laboratory | SIEMENS energy | GEFERTEC | PITT MOST-AM Modeling & Optimization Simulation Tools for Additive Manufacturing

- ❑ AM process similar to direct energy deposition
- ❑ Uses an electric arc as the heat source
- ❑ Solid wire as feedstock material
- ❑ Main advantage is its high deposition rates and minimal wastage of material
- ❑ Low running cost and short production cycle
- ❑ It can produce large metallic parts
- ❑ Main disadvantage is the precision of as-built parts may be lower than those by powder-bed systems



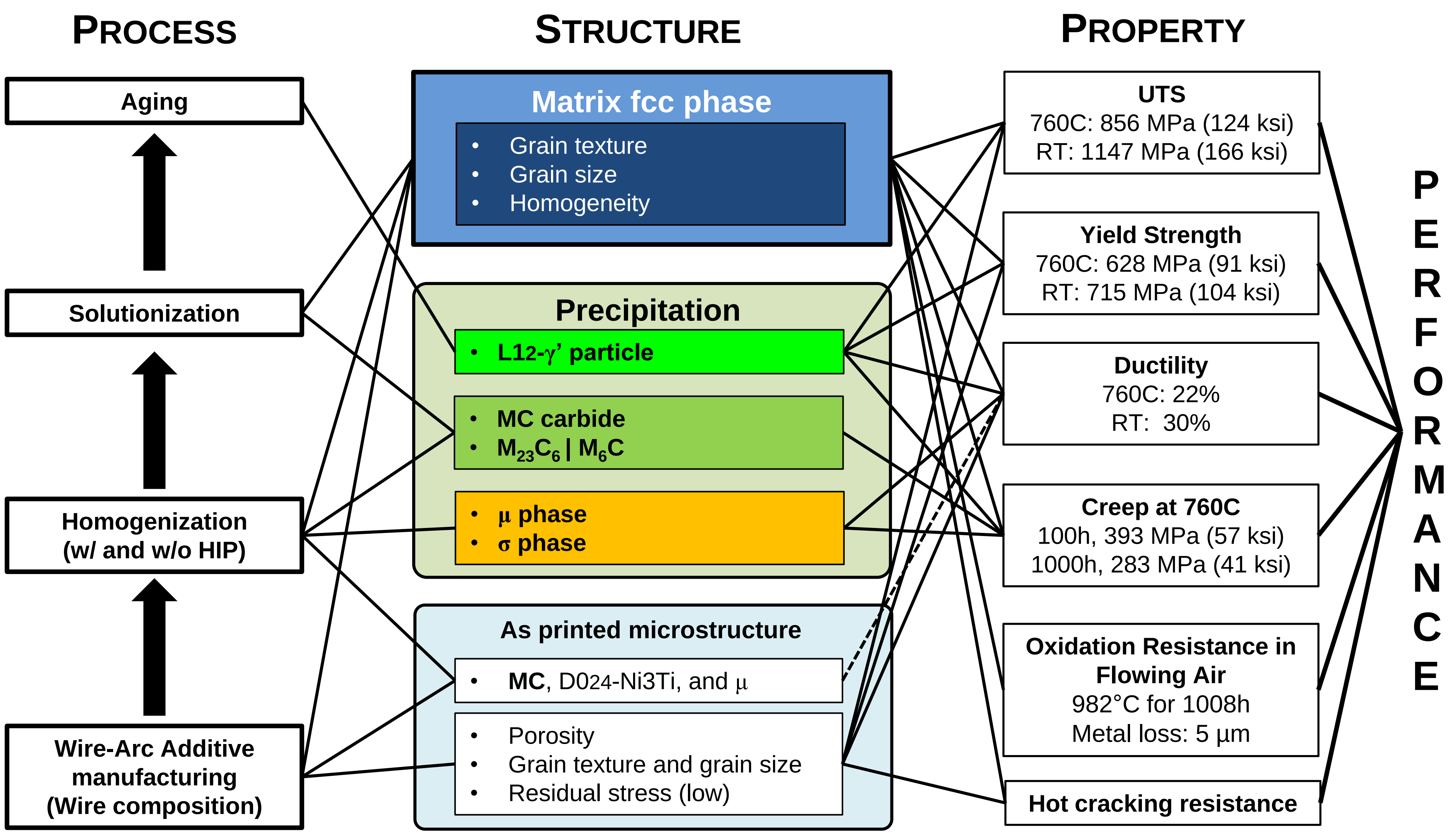
T.A. Rodrigues, Materials. 12 (2019).



GEFERTEC arc605

ARC 605 : 5-axis machining: Production of metallic components up to 0.8 m³ with a maximum mass of 500 kg.

Systems Design Chart for Haynes 282



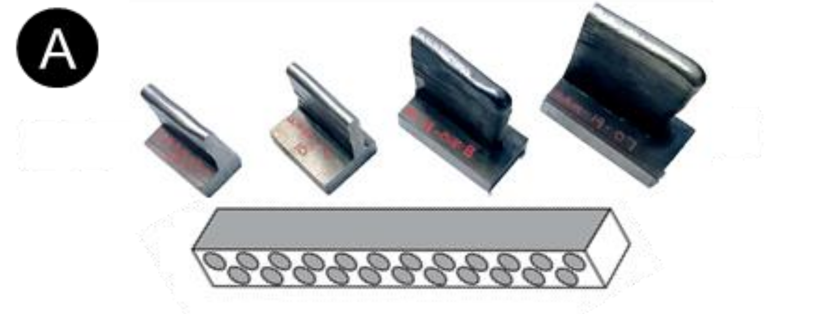
Planned studies in this project

ICME modeling enhanced by machine learning

- **A1.** As-print microstructure study on WAAM HAYNES 282
- **A2.** Recrystallization study on WAAM HAYNES 282
- **A3.** HT Aging study on WAAM HAYNES 282

B1. Location specific microstructure respond based on processing parameters (print + heat treatment)

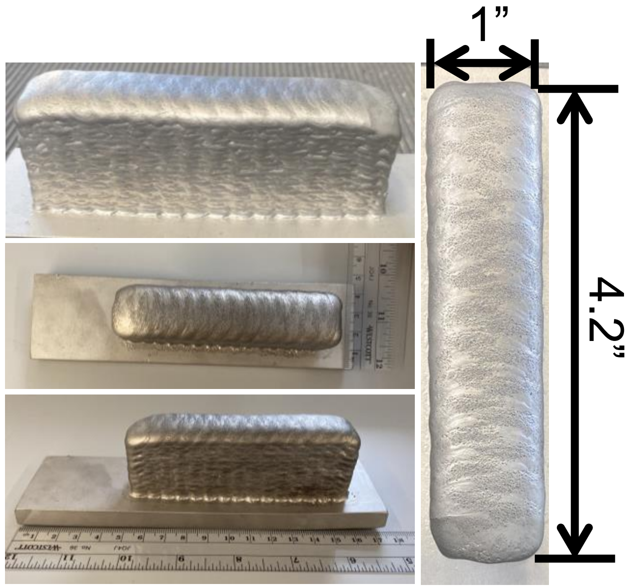
Shape effect:
Height & Cross section



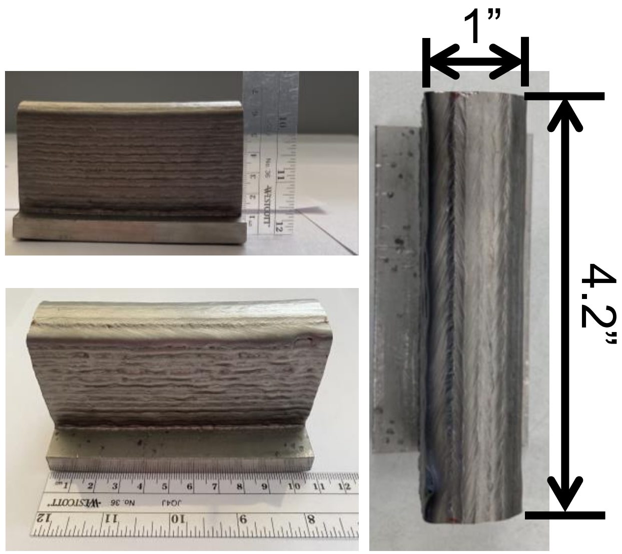
HT WAAM sample with gradient temperature and processing parameter

Complex geometry build for location specific ICME design

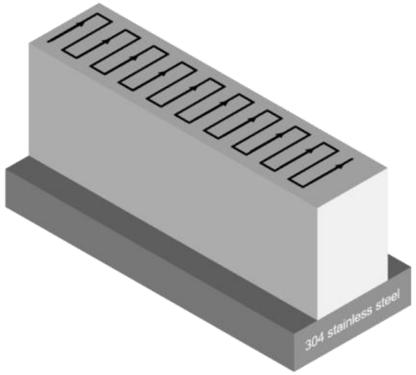
Printing strategy difference: Meander vs. Single Bead



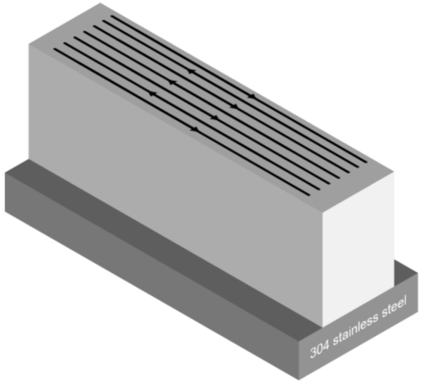
Multitrack Meander Haynes 282



Multitrack Single Bead Haynes 282

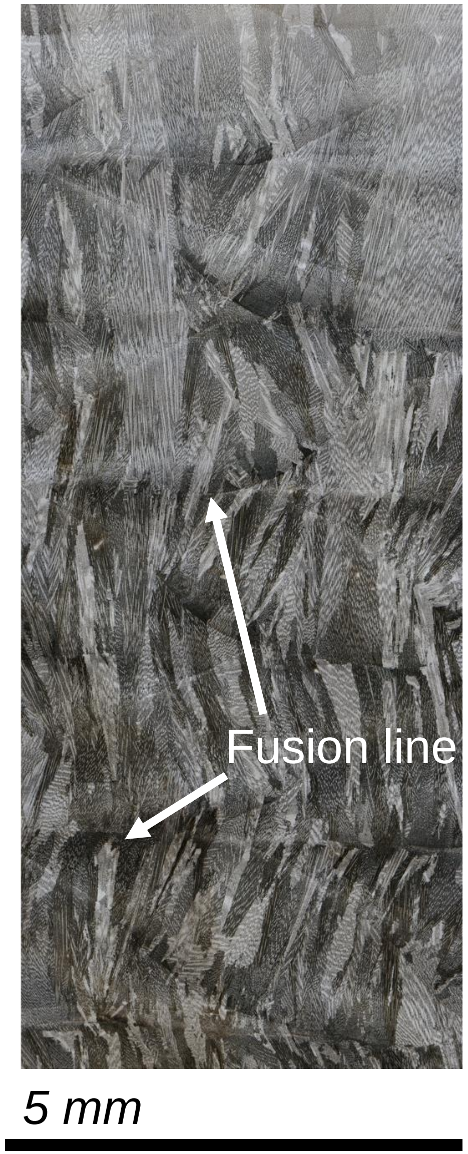


Zigzag, Meander



Single bead

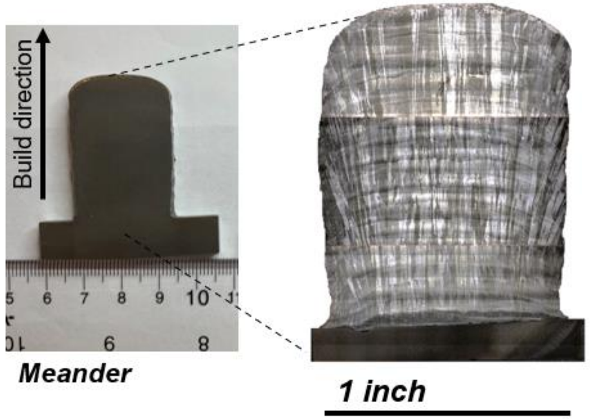
As-printed microstructure: Meander vs. Single Bead

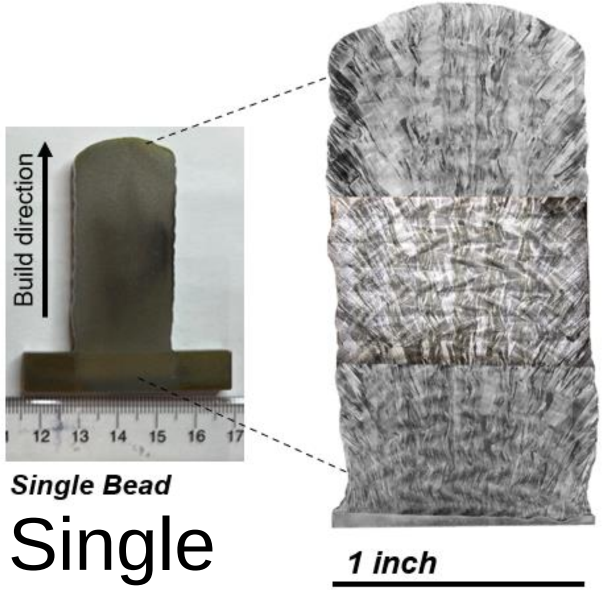


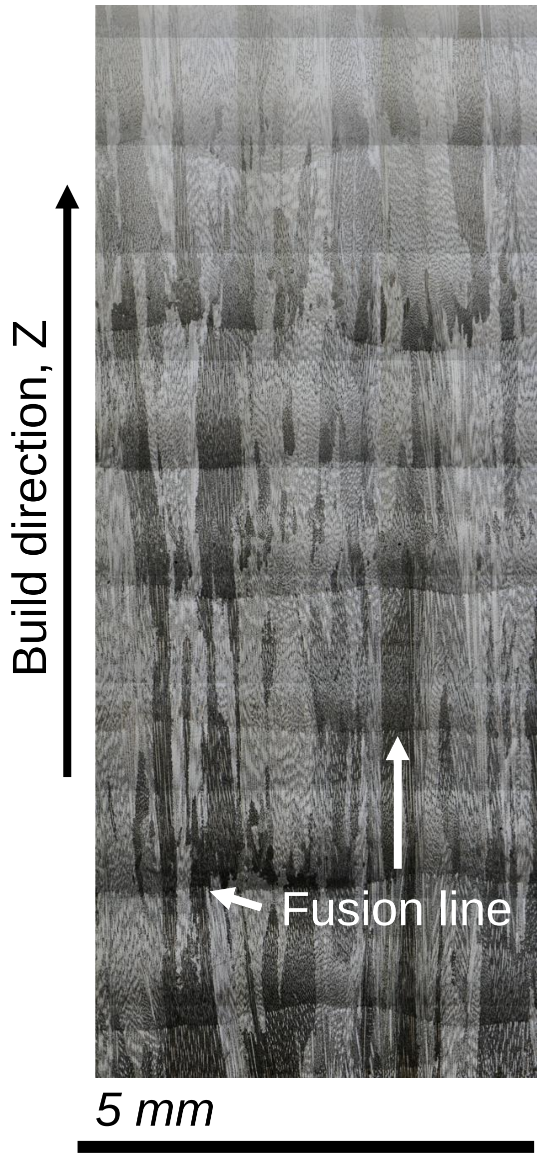
Zig-zag (meander)

vs.

Single bead

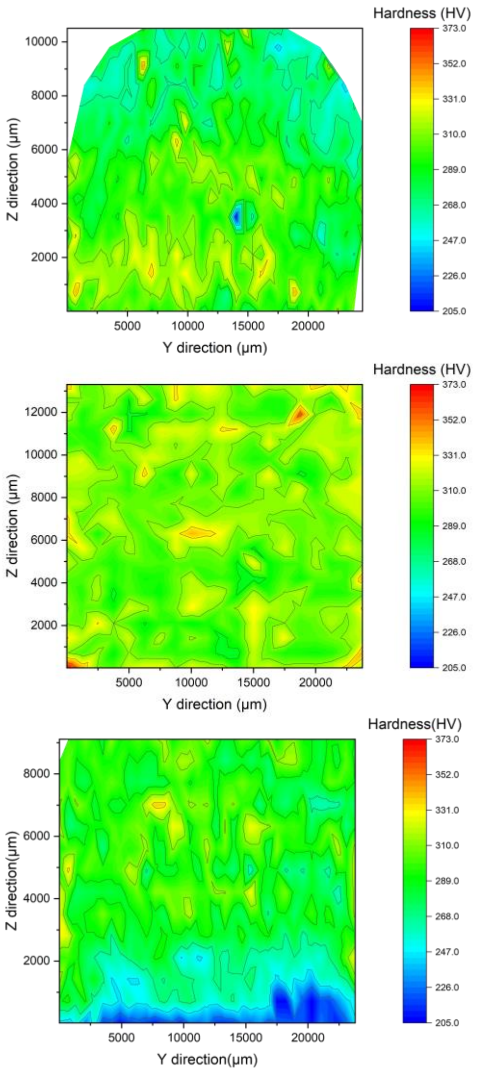


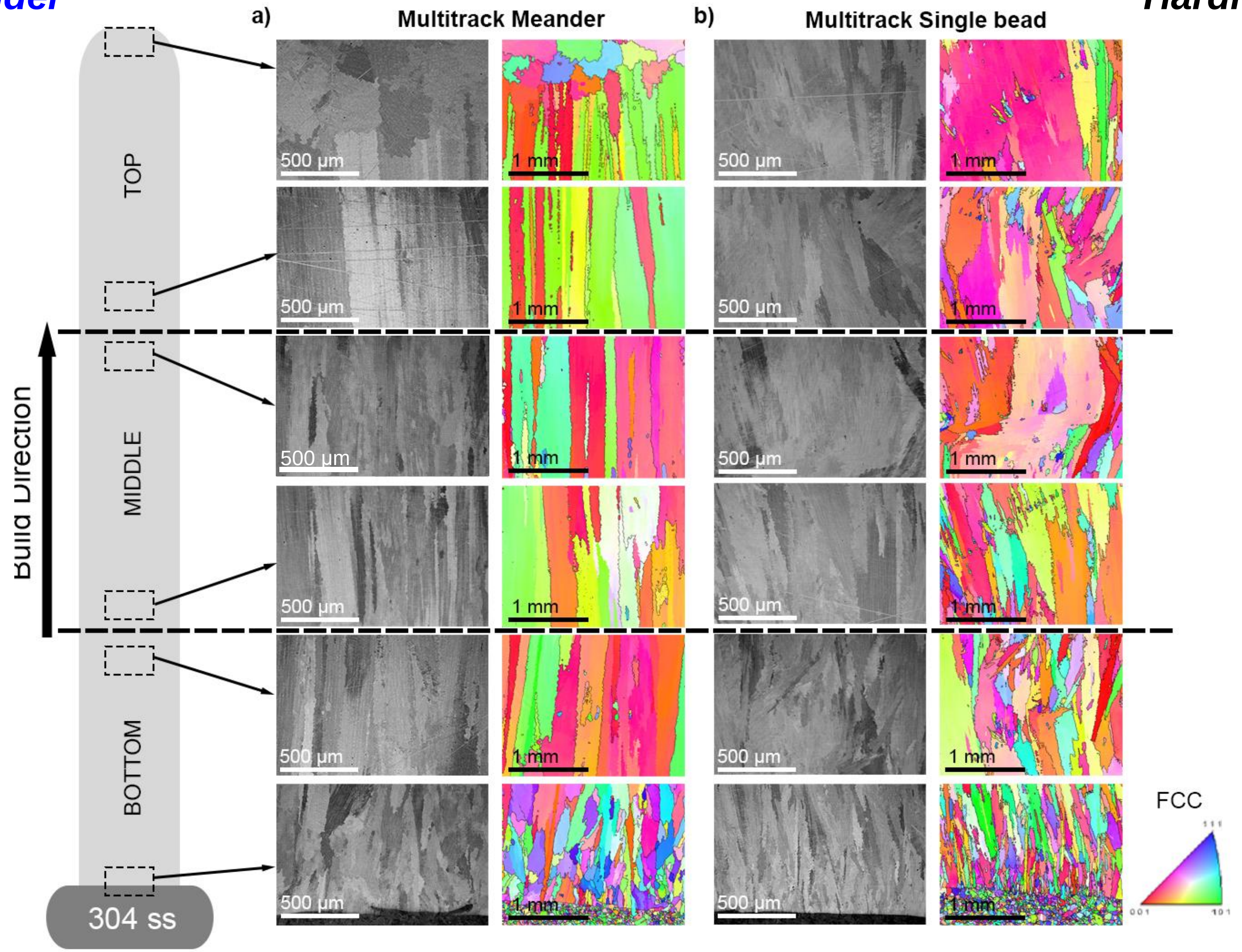




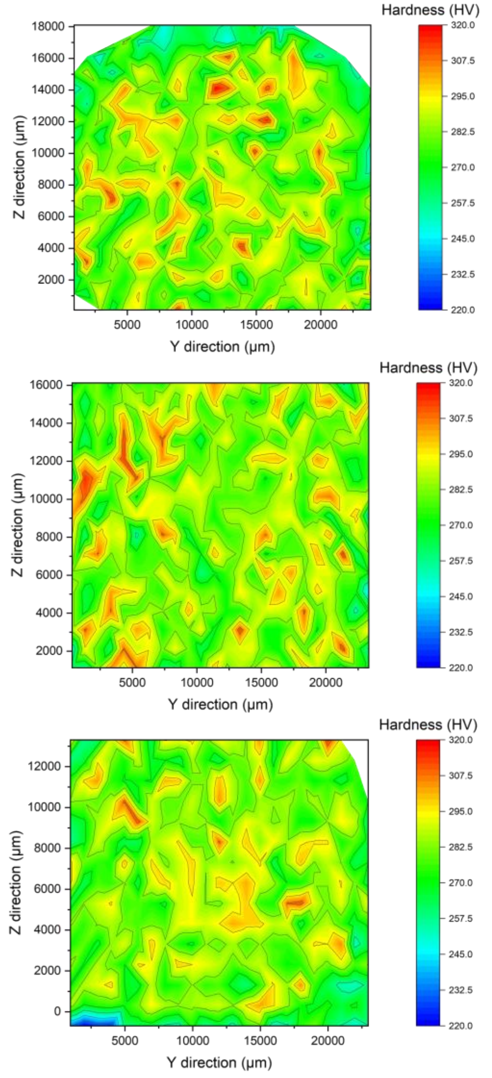
As-printed microstructure : Meander vs. Single Bead

Hardness Map of Meander

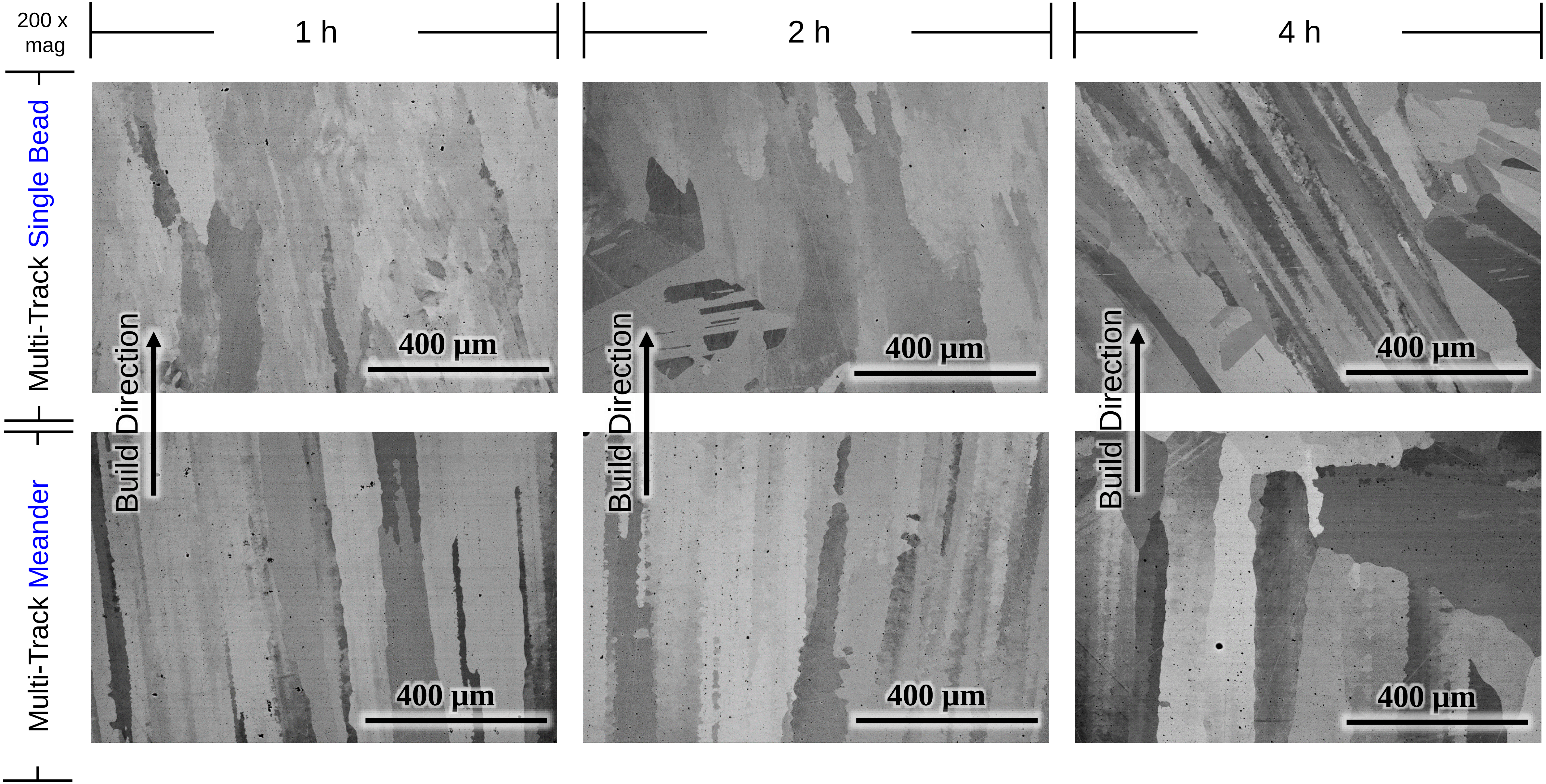




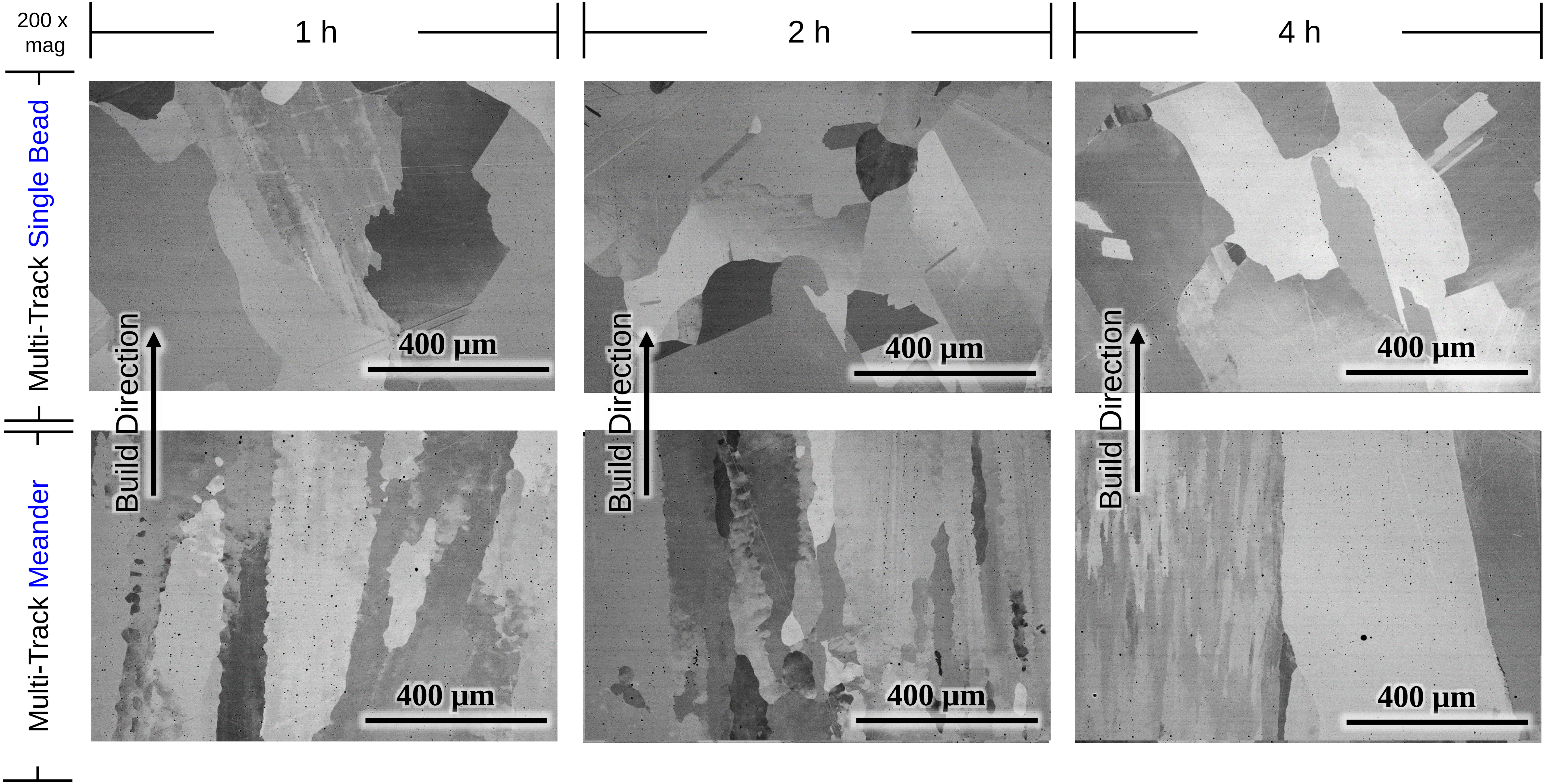
Hardness Map of Single Bead



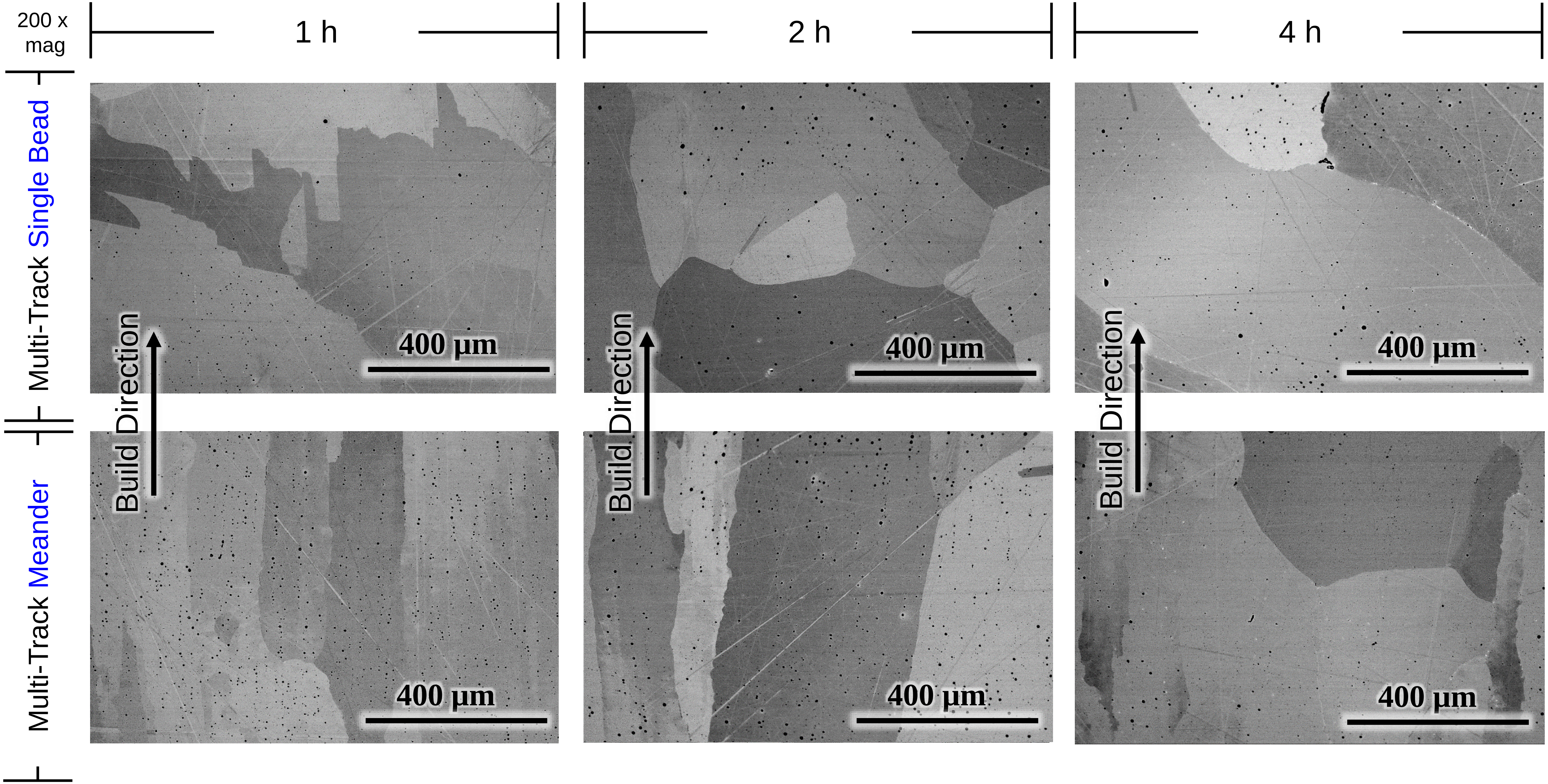
Haynes 282: Meander *vs.* Single Bead (Recrystallization at 1200°C)



Haynes 282: Meander *vs.* Single Bead (Recrystallization at 1250°C)



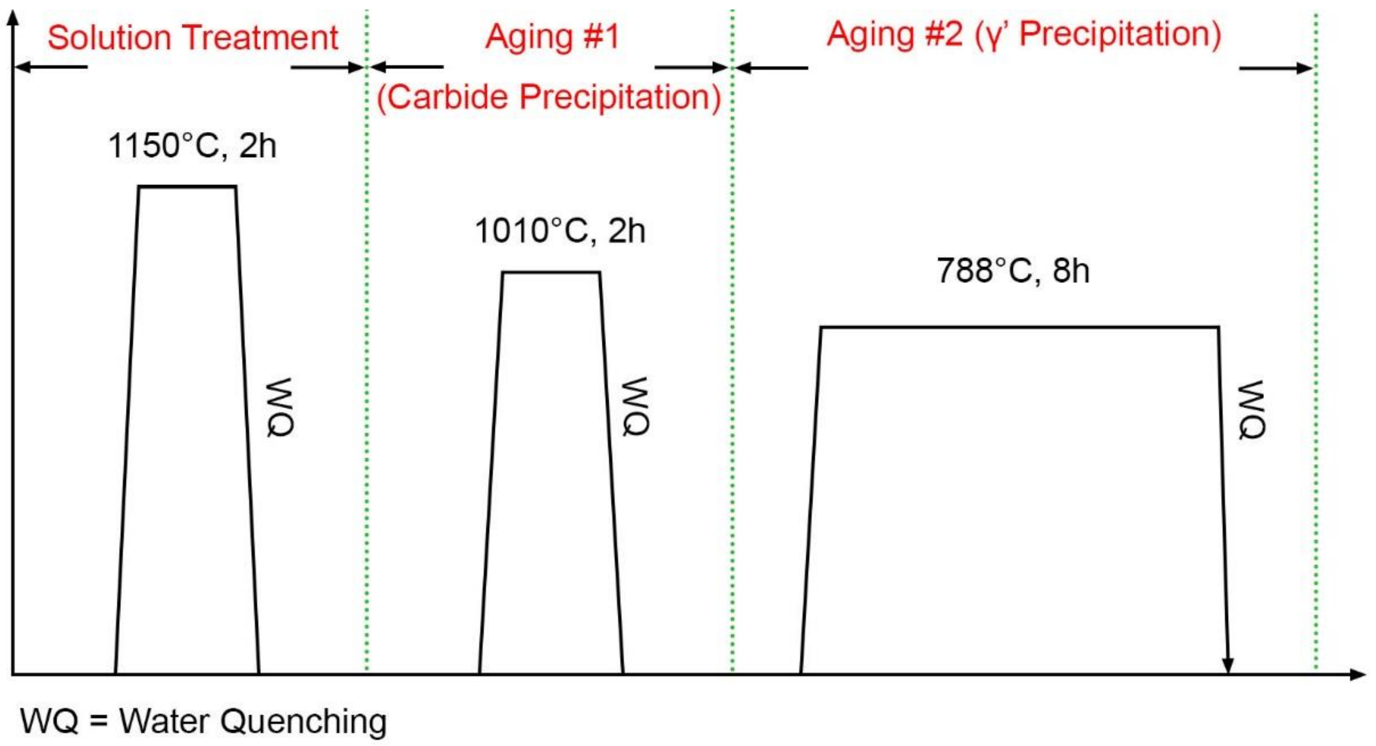
Haynes 282: Meander *vs.* Single Bead (Recrystallization at 1300°C)



Experimental Procedures

- Aging #1 induces the precipitation of M23C6 carbides
- Aging #2 is responsible for the precipitation of the γ'
- Water quenching is performed at the end of each heat treatment stage to accurately control the precipitation kinetics
- 4 samples: as-printed, solutionized, after aging #1 and after aging #2

Recommended heat treatment for cast Haynes 282 alloys

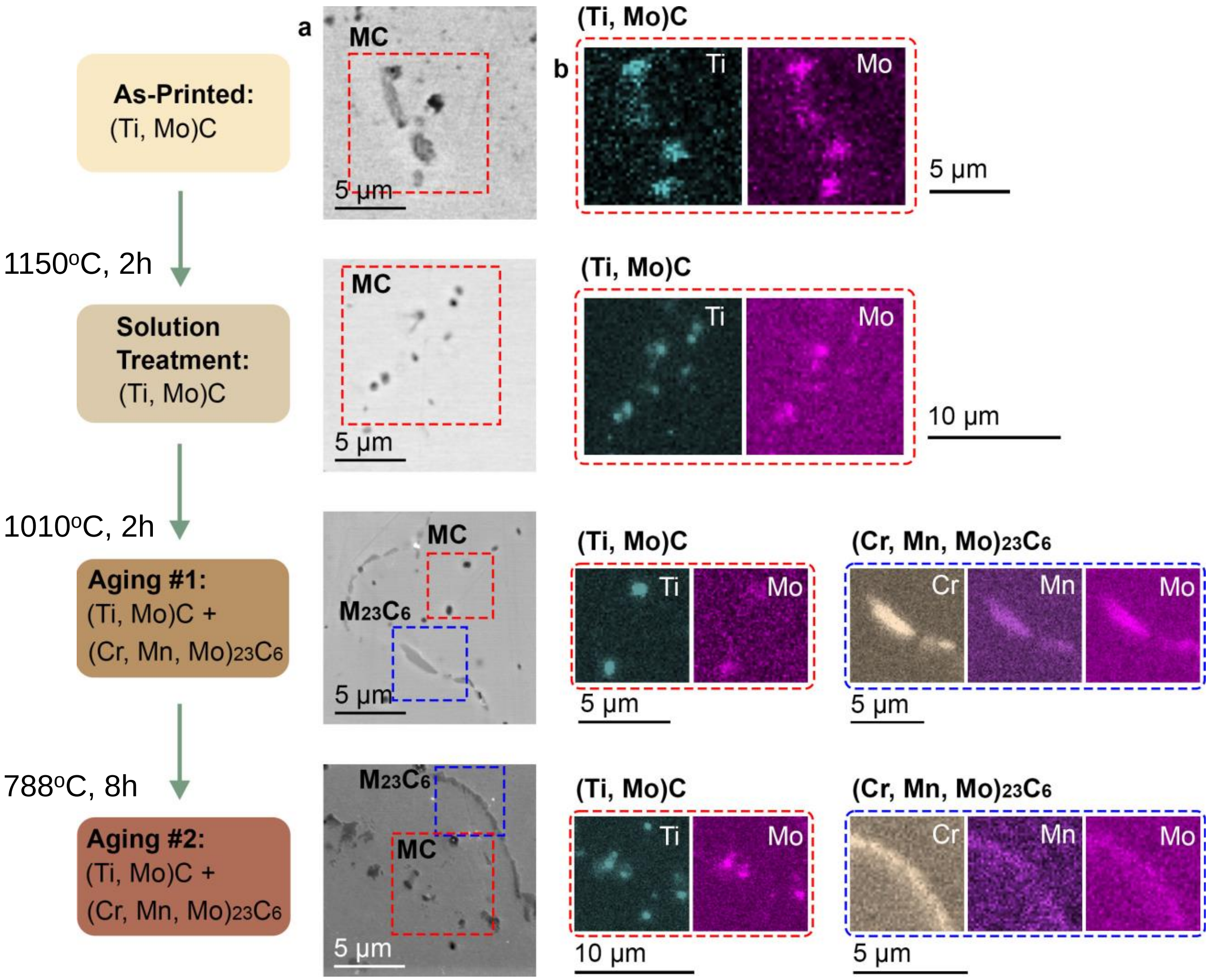


Evolution of Carbides as a Function of Heat Treatments

- Combined analysis with secondary electron (**SE**) and **EDS** mapping

- (Ti, Mo)C carbides are 1~5 μm in the as-printed sample and reduced to ~1 μm after solution treatment. They remain almost unchanged in the subsequent aging treatments.

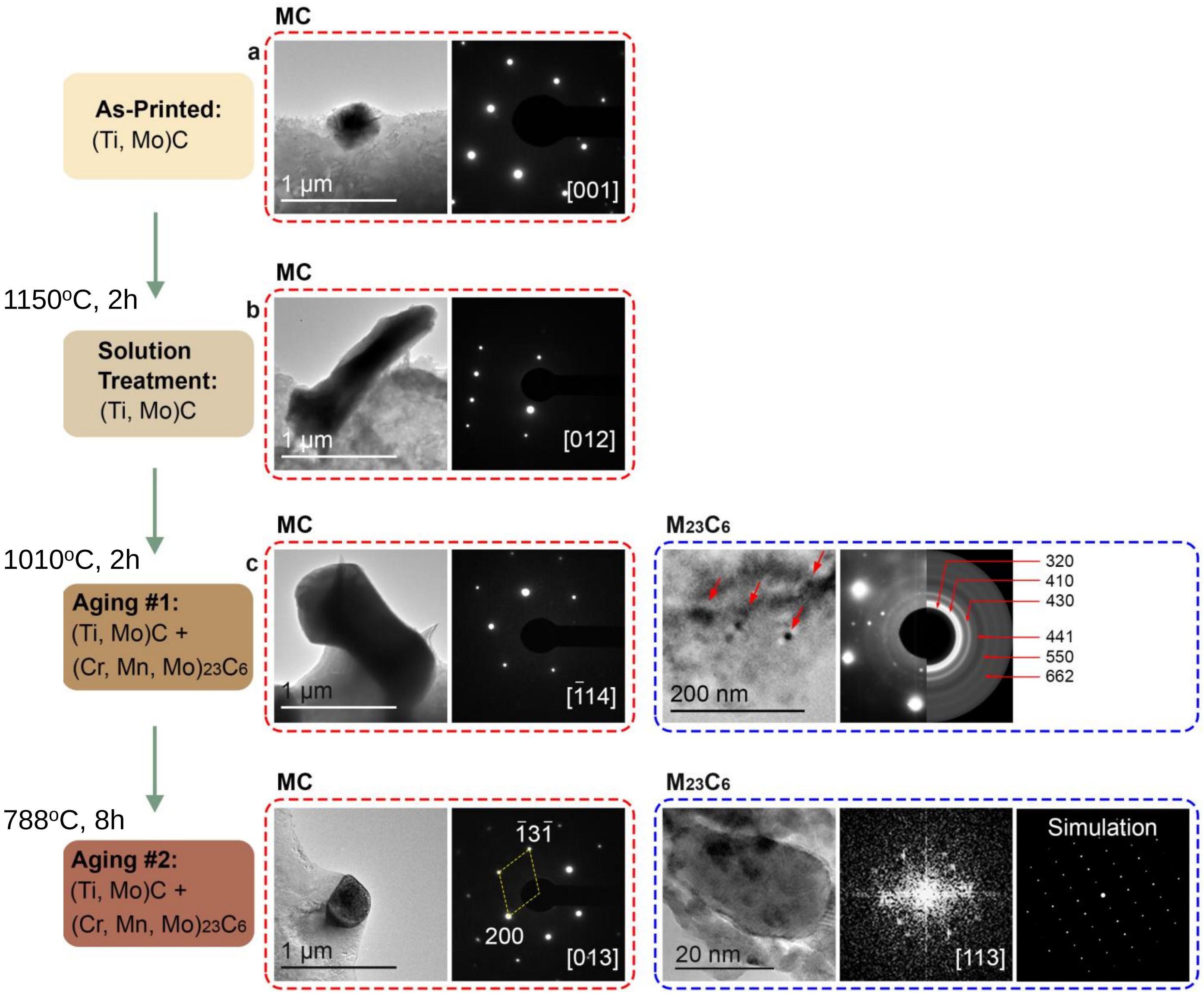
- The (Cr, Mn, Mo)$_{23}$C$_6$ carbide shows up on the grain boundaries after the aging #1. They look almost unchanged after aging #2.



Phase Identification with Electron Diffraction

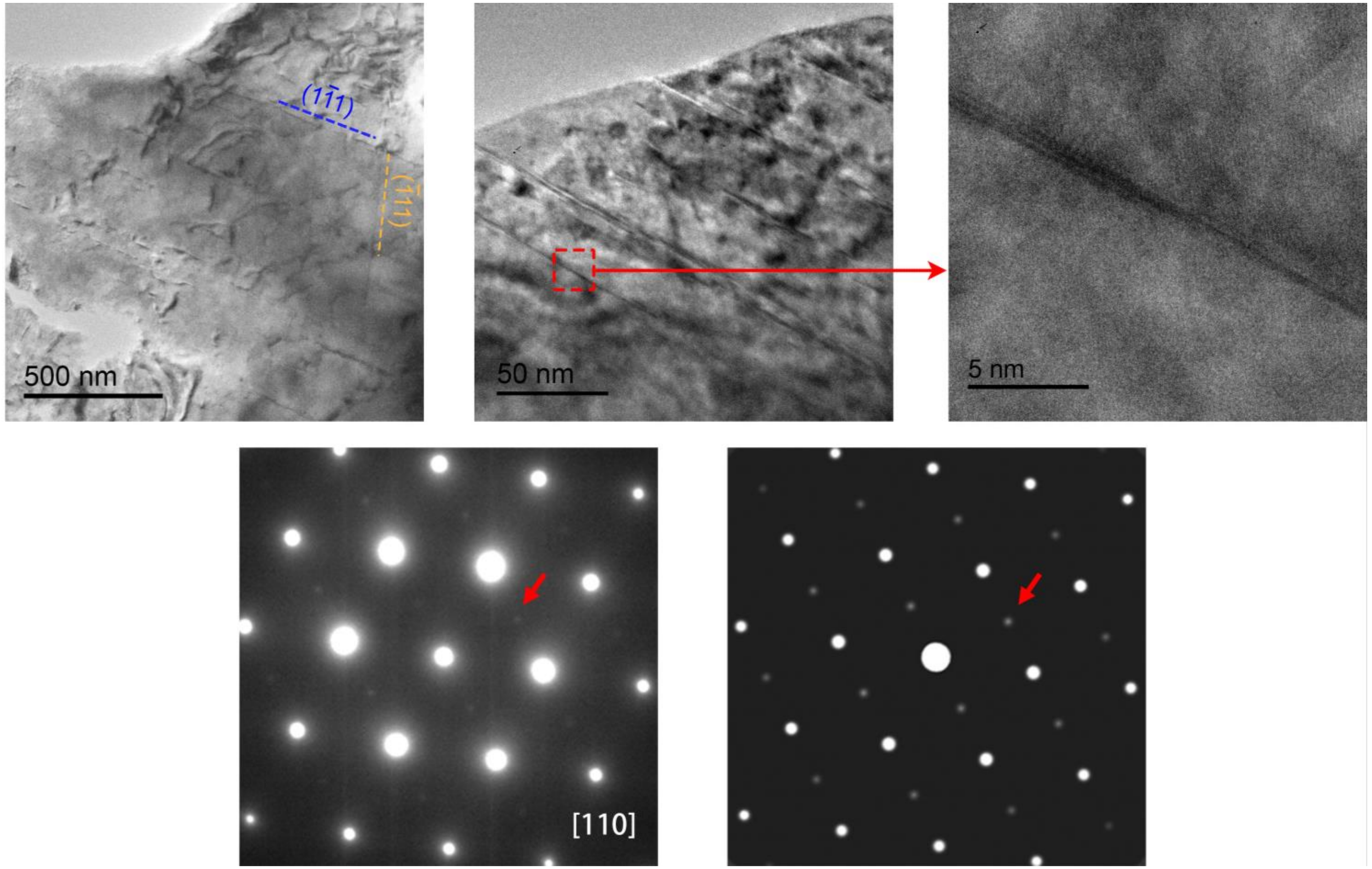
- The (Ti, Mo)C and (Cr, Mn, Mo)$_{23}$C$_6$ phases shown in the last slide are confirmed with **TEM** bright-field imaging along with **electron diffraction**.
- The *Fm*$\bar{3}$*m* structures (F.C.C.) of the (Ti, Mo)C and (Cr, Mn, Mo)$_{23}$C$_6$ carbides are confirmed.
- The lattice constants of the (Ti, Mo)C and (Cr, Mn, Mo)$_{23}$C$_6$ carbides closely match with the previous reports.

1. *Mater. 6 (2013) 5016–5037.*
2. *Crystals 2021, 11(8), 867*



γ’ Precipitation in the As-Printed Material

- γ’ needles/thin plates are present in the as printed material
- The widths of the needles are 1~2 nm (a few atomic layers)
- The needles are found along the {111}-type atomic planes



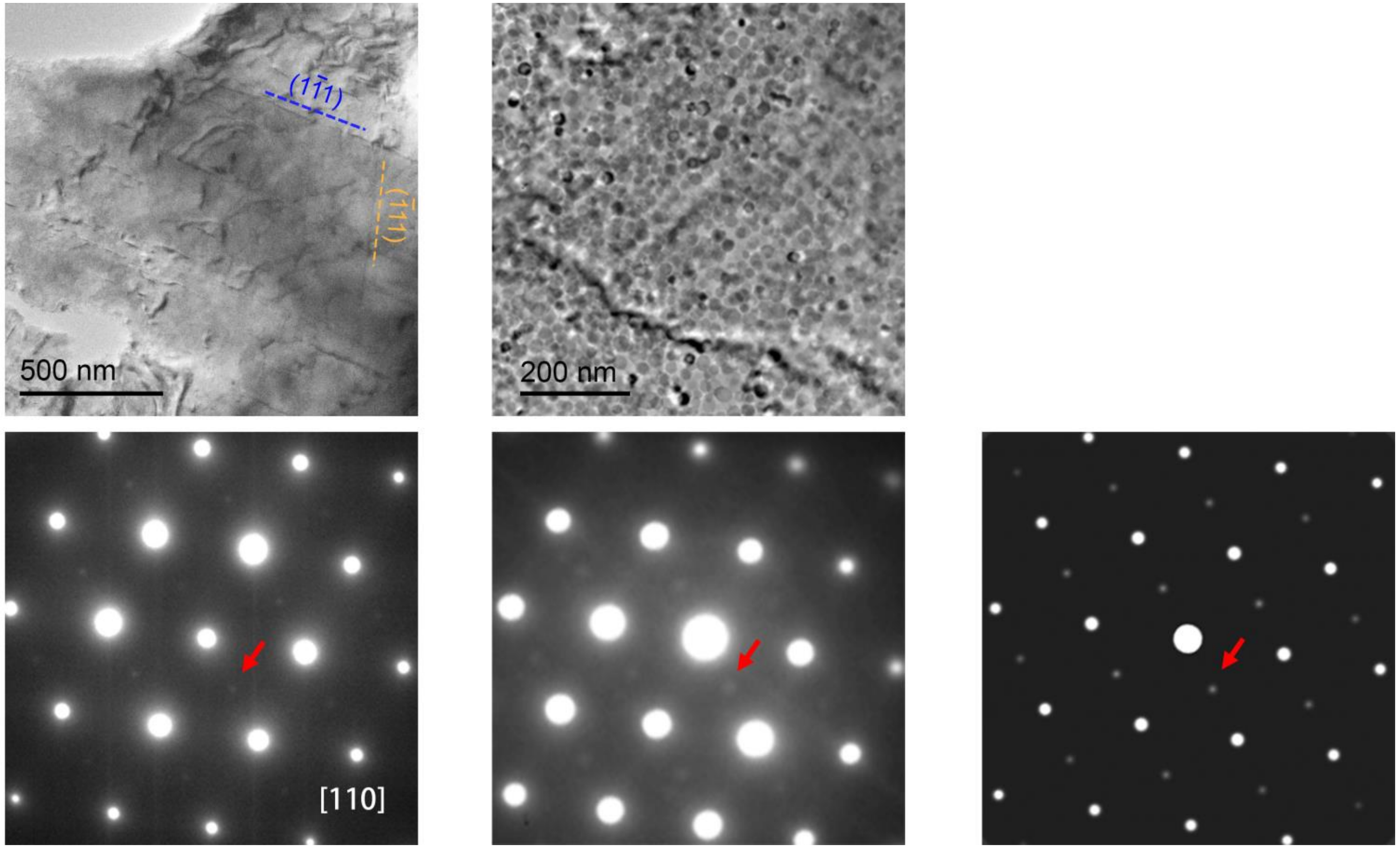
γ’ Evolution with the Heat Treatments

- γ’ needles are found in the as printed sample, and γ’ spheres are present in the one after full heat treatments .
- The presence of γ’ precipitates are confirmed with electron diffractions.
- The γ’ needles have coherent or semi-coherent interfaces with the γ matrix, and the γ’ spheres have incoherent interfaces against the matrix.

As-Printed: γ’ needles

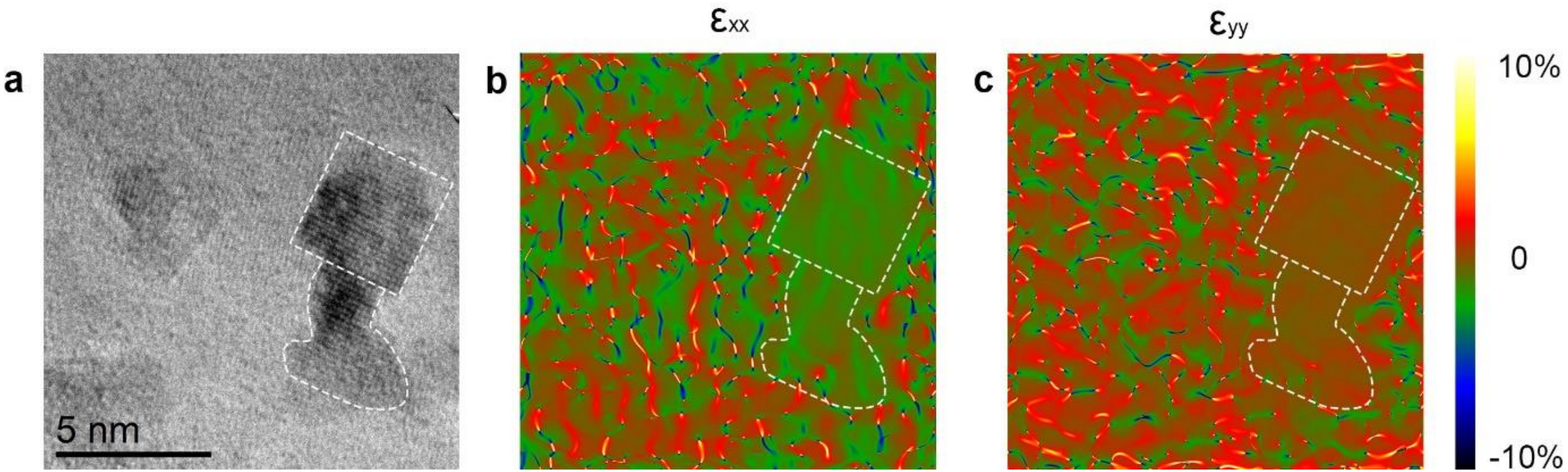
1150°C, 2h + 1010°C, 2h + 788°C, 8h

Diffraction Simulation



Nucleus of γ’

1150°C, 2h + 1010°C, 2h + 800°C, 6h



- Nucleus of the γ’ phase from the γ matrix is around 3~5 nm.
- Intensive internal stress in generated within the γ matrix while almost no stress in present in the γ’ phase, confirming the γ/γ’ lattice mismatch and softer nature of γ compared with γ’.

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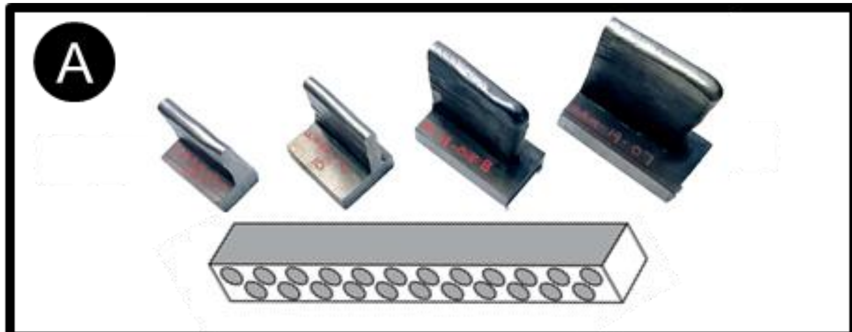
B1. Location specific microstructure respond based on processing parameters (print + heat treatment)

Shape effect:
Height & Cross section



HT WAAM sample with gradient temperature and processing parameter

Complex geometry build for location specific ICME design

Data bank collection for location specific microstructural analysis (ML)

Location	Printing Parameters		Composition Variation [wt.%]	Experimental Variables		Modeling Variables	
Height (Z): Top | Middle | Bottom **Radius (±R) :** Left | Center | Right	Printing Pattern Layer Thickness Interlayer temperature Interlayer Idle time	Voltage/Current Pulse Power Wire Feed Rate Torch Traveling Speed & Working Distance Shielding Gas	Ni, Co Ti, Al Nb, Cr, Mo C, B Fe, Mn, Si	Phase fraction & composition Precipitate size Grain Size & morphology Dislocation Density Residual Stresses Texture	Vickers Hardness	Phase fraction & composition Precipitate size Liquidus Solidus Freezing Rage TEC, α Latent heat, L	Yield Strength Vickers Hardness

Input for ICME/ML models

ICME framework for Modeling Variables

As-printed Microstructure

Scheil-Gulliver predictions
of phase fraction and composition

Post-heat-treated Microstructure

Equilibrium predictions
of phase fraction and composition

Yield Strength & Hardness model

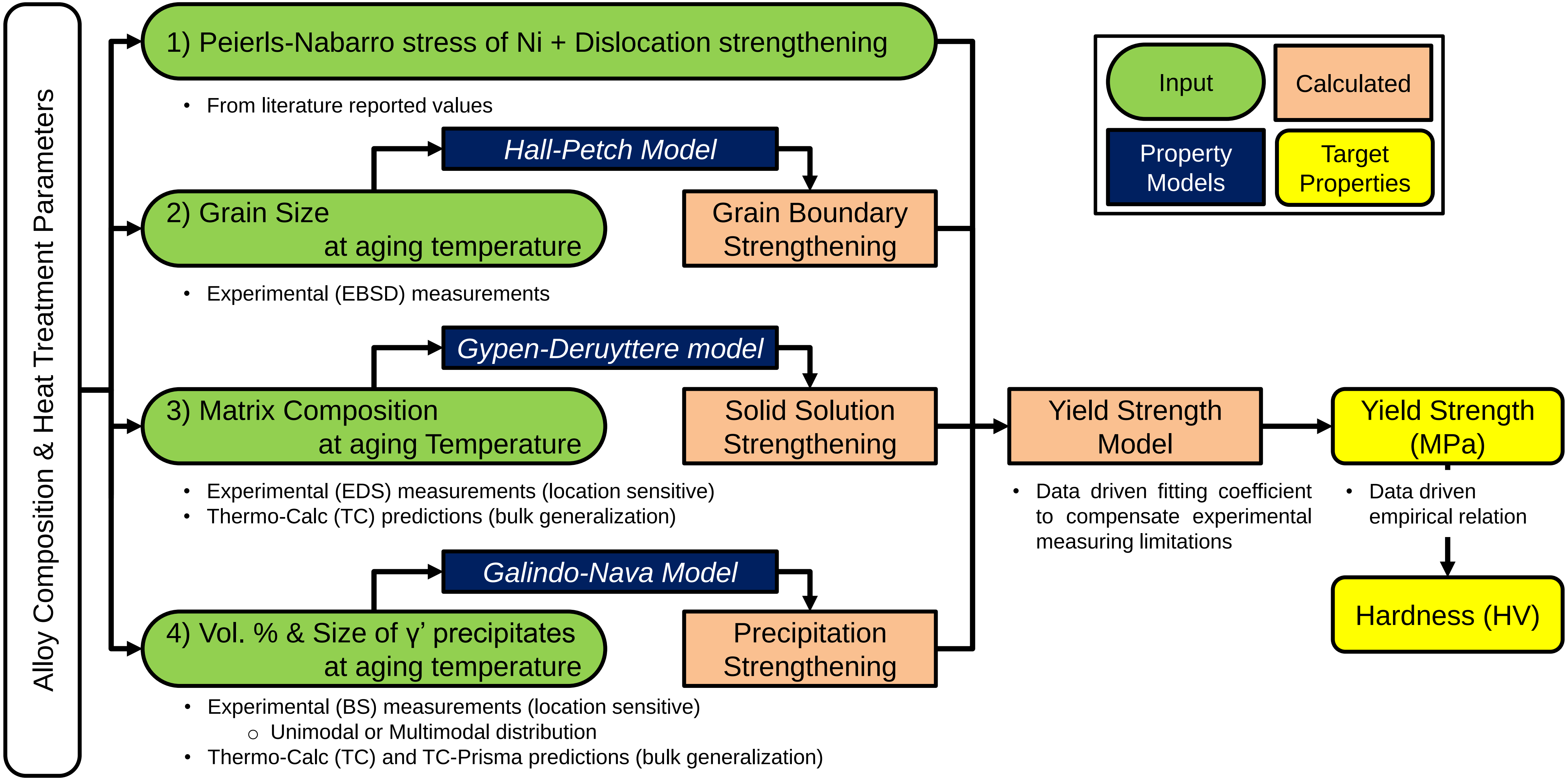
Solidification Properties

Heat Capacity, Cp
Latent Heat, H_L
Thermo Expansion Coefficient, TEC

Printability Index

Liquidus, Solidus and
Freezing Range

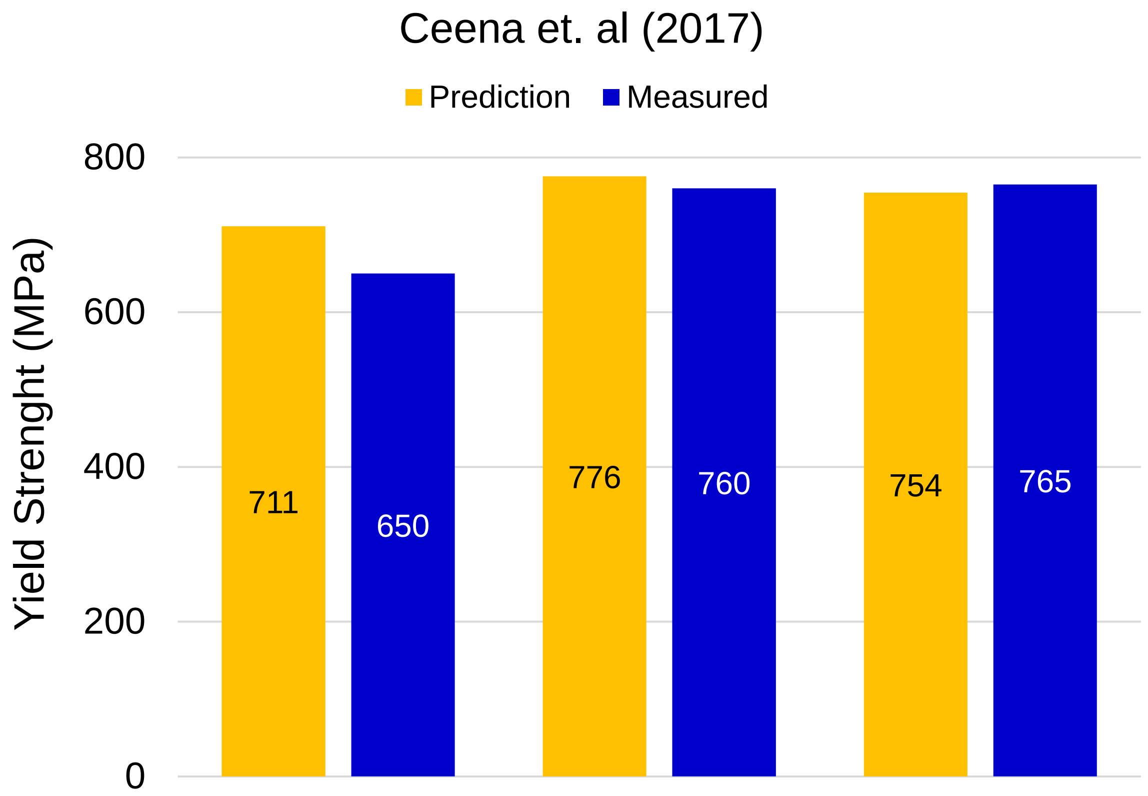
Modeling Framework: Yield Strength Model



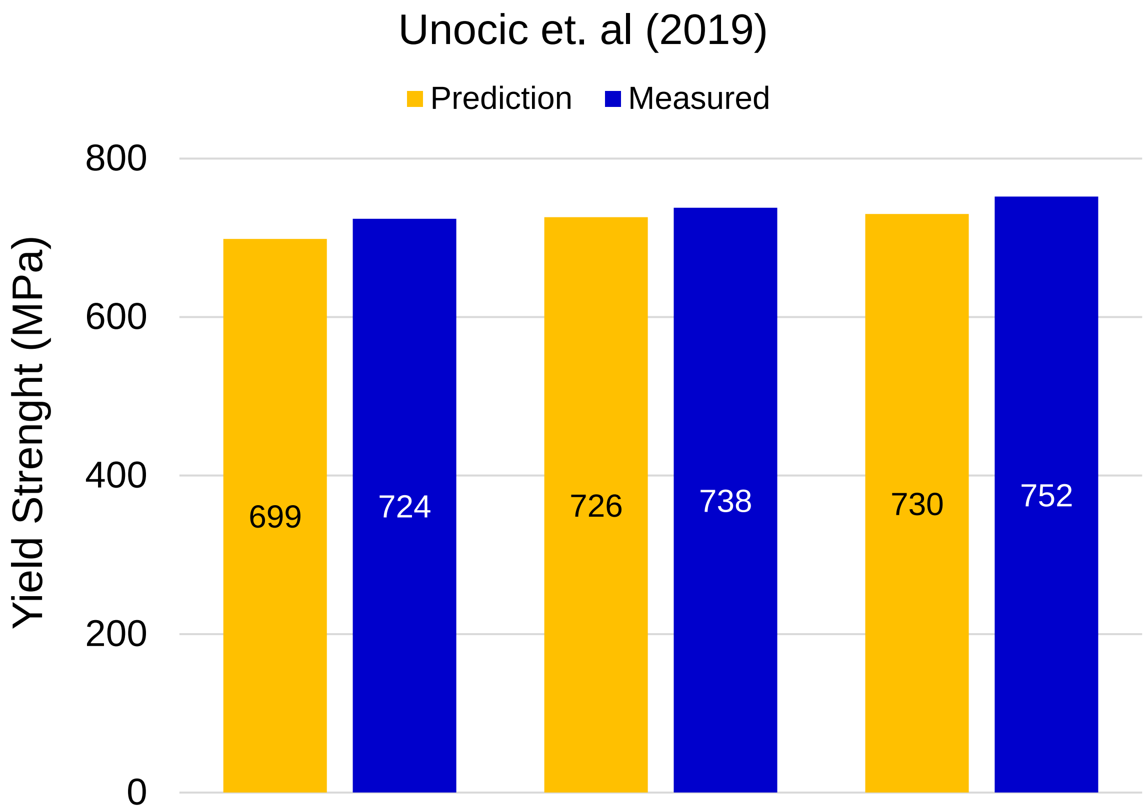
Room Temperature Yield Strength Model: Calibration with cast HAYNES 282

Power Fitted Yield Strenght Model: $\sigma_{yield} = ({\sigma_{PN}}^{k} + {\sigma_{GS}}^{k} + {\sigma_{SS}}^{k} + {\sigma_{P}}^{k})^{1/k}$, $\boldsymbol{k = 1.0}$

Average Error $= \mathbf{3.16 \pm 2.87}$



Annealed:	1120 °C/ 2h	-	-
1st Aging:	1010 °C/ 2h	1010°C/ 2h	996 °C/ 2h
2nd Aging:	788 °C/ 8h	788 °C/ 8h	788 °C/ 8h

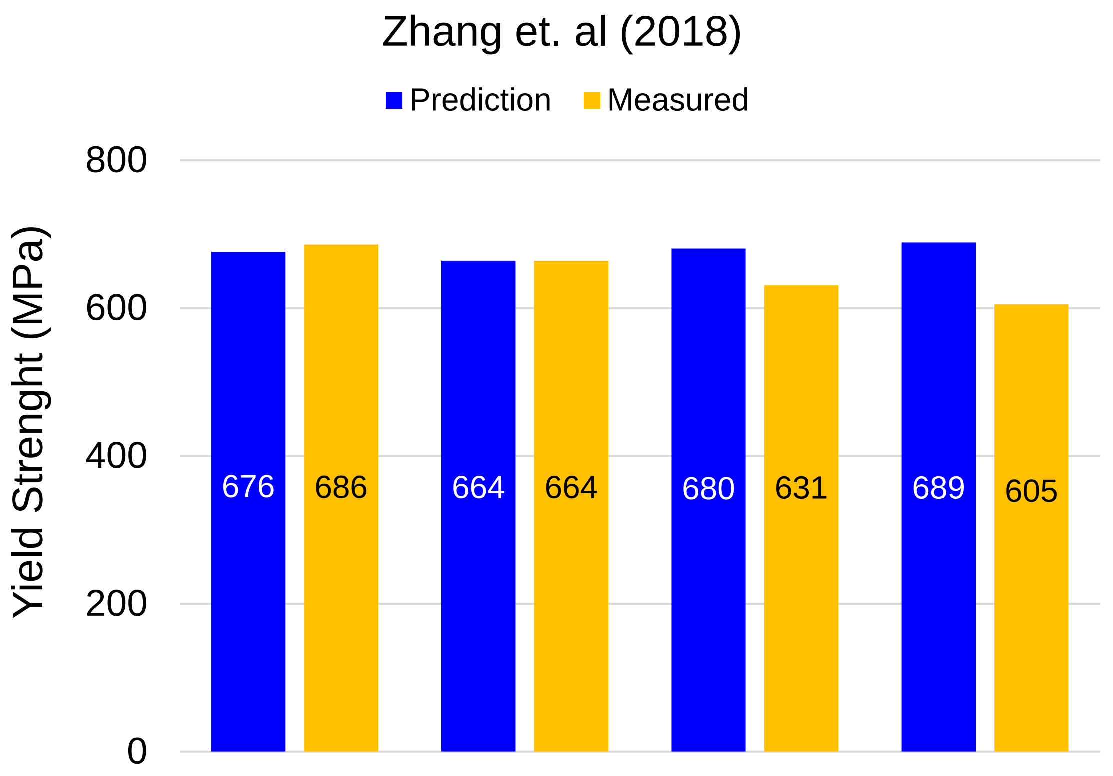


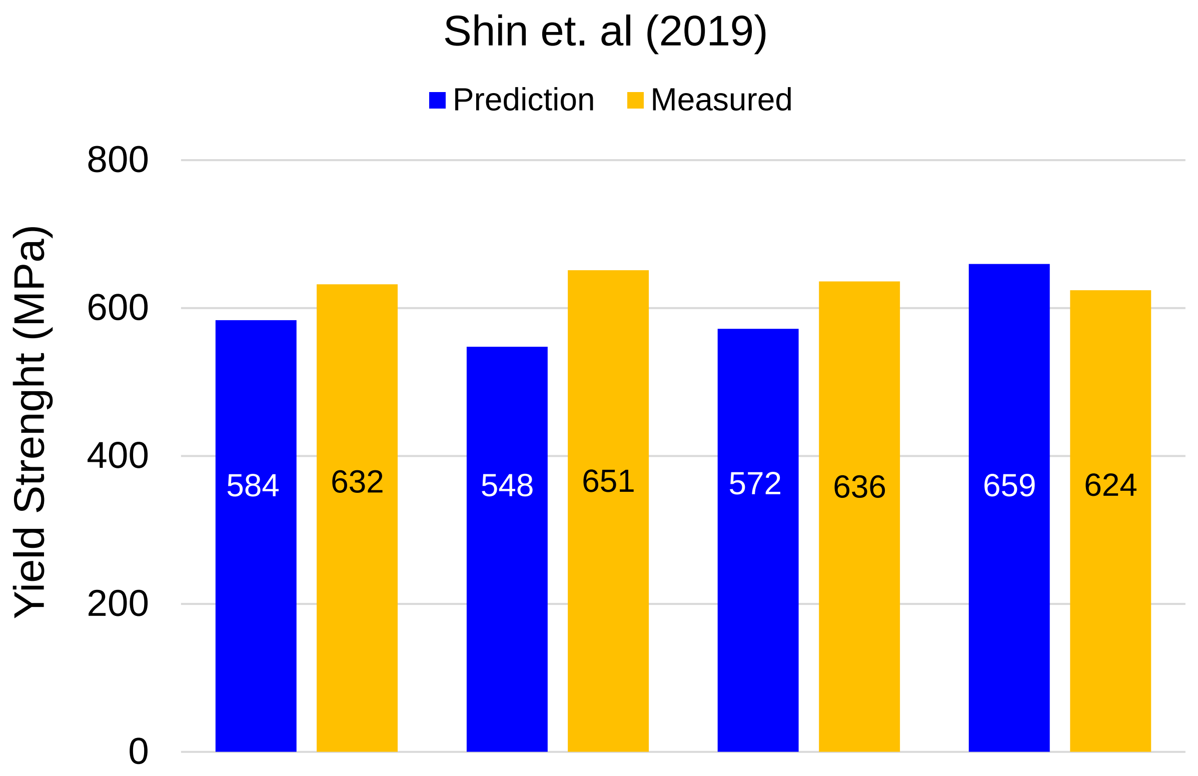
Annealed:	Commercial solution treatment (1121 – 1149 °C)		
1st Aging:	800 °C/ 4h	800 °C/ 6h	800 °C/ 8h

High Temperature Yield Strength Model: Calibration with cast HAYNES 282

Power Fitted Yield Strenght Model: $\sigma_{yield} = ({\sigma_{PN}}^{k} + {\sigma_{GS}}^{k} + {\sigma_{SS}}^{k} + {\sigma_{P}}^{k})^{1/k}$, $\boldsymbol{k = 1.06}$

Average Error $= \mathbf{7.26 \pm 3.60}$

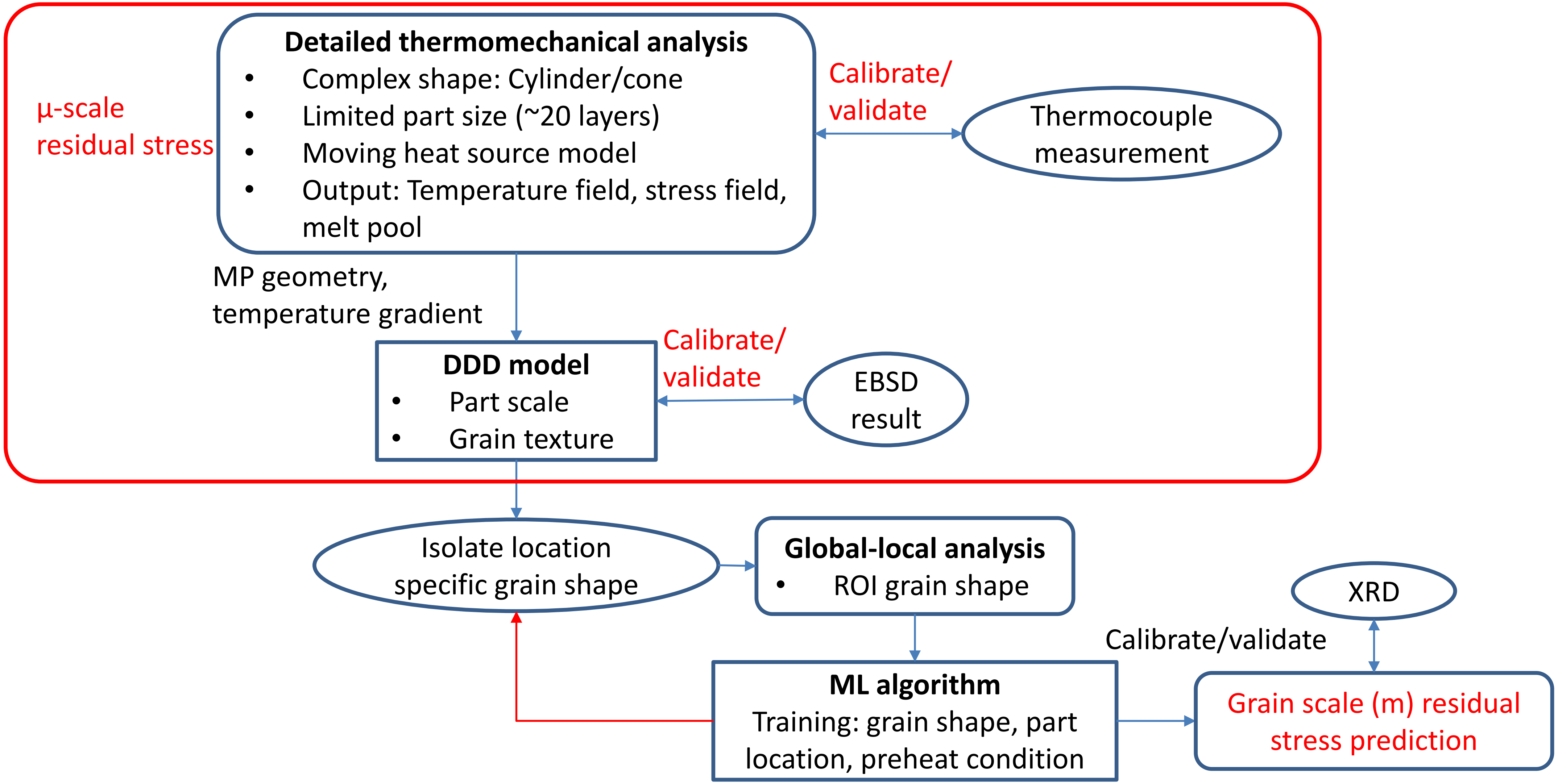




Annealed: ---------------------1140 °C/2h AC-----------------
-1st Aging: ---------------------1010 °C/2h AC-----------------
2nd Aging: --------------------- 760°C/24h AC----------------
Test Temp: 600 °C 700 °C 760 °C 800 °C

Annealed: 1135°C/20min WQ AC FC
-1st Aging: 1010 °C/2h - - -
2nd Aging: 788°C/8h 800C/4h 800C/4h 800C/4h
Test Temp: -----------------------750 °C------------------------------

Part scale residual stress prediction: Flowchart

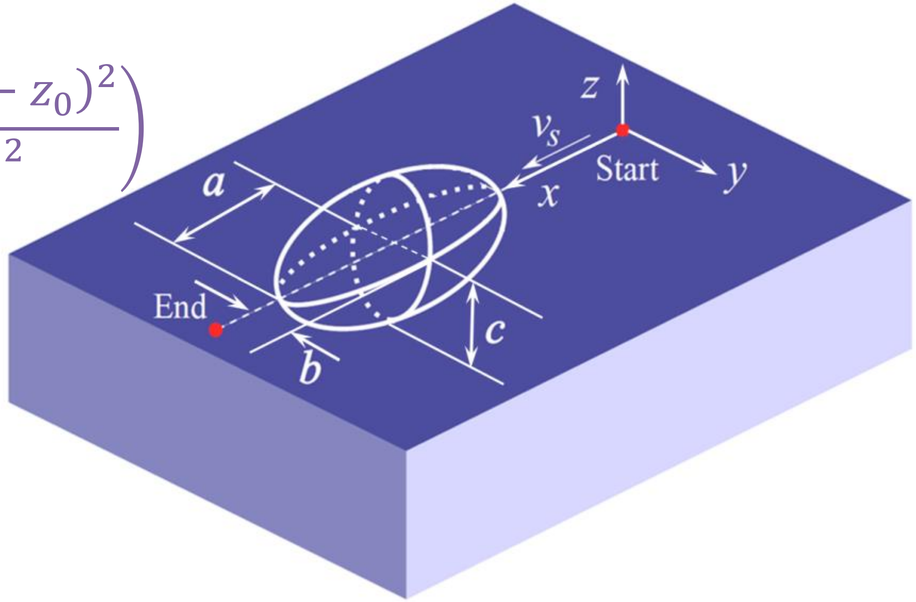


Thermal property requirements

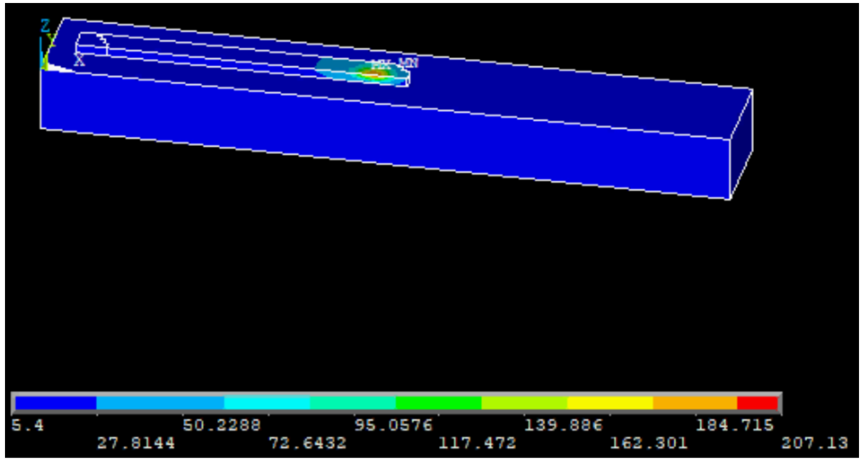
- 3D heat conduction equation: $\boldsymbol{\rho C_p}\left(\frac{\partial T}{\partial t} + U_i\, \nabla T\right) = \nabla(\boldsymbol{K}\, \nabla T)$
- Thermal boundary condition: $\boldsymbol{K}\frac{\partial T}{\partial n} + h(T - T_0) + \sigma\varepsilon(T^4 - T_0^4) - \dot{Q} = 0$
- Initial and final condition: $T(x, y, z, 0) = T_0 = T(x, y, z, \infty)$
- In the simulation, the heat source is represented by the **double ellipsoidal heat source model** with $\dot{Q}$ is defined as follows,

$$\dot{Q} = \frac{6\sqrt{3}\eta P f}{abc\pi\sqrt{\pi}} exp\left(-\frac{3(x_0 + v_s t - x')^2}{a^2} - \frac{3(y' - y_0)^2}{b^2} - \frac{3(z' - z_0)^2}{c^2}\right)$$

Parameters a, b, c obtained by calibrating the double ellipsoidal heat source model



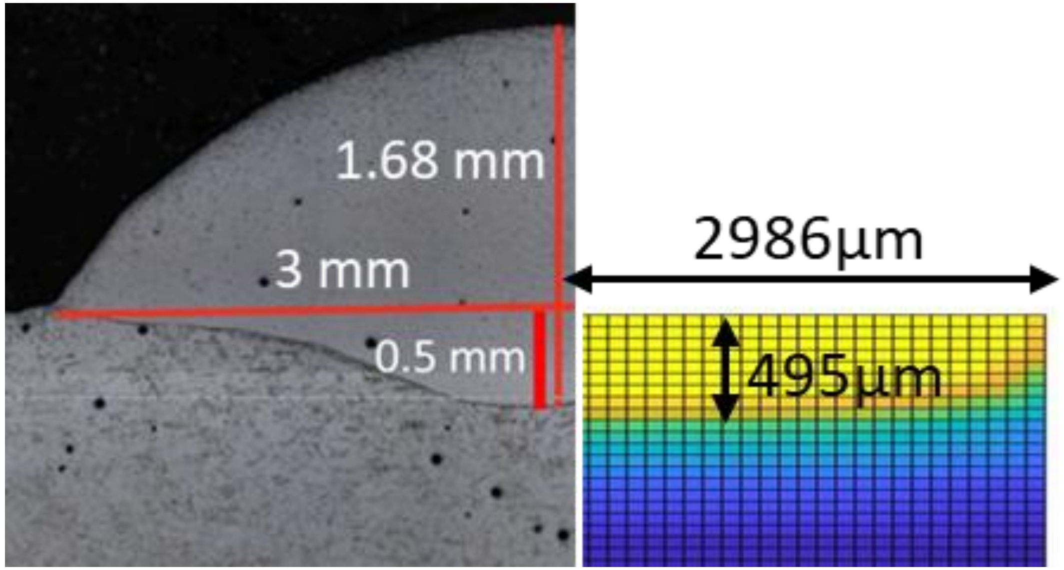
Heat source calibration: Single track



Temperature distribution from FE model for single track deposition

$$a = 10, b = 40, c = 0.6$$

Dimensions of single-track deposition

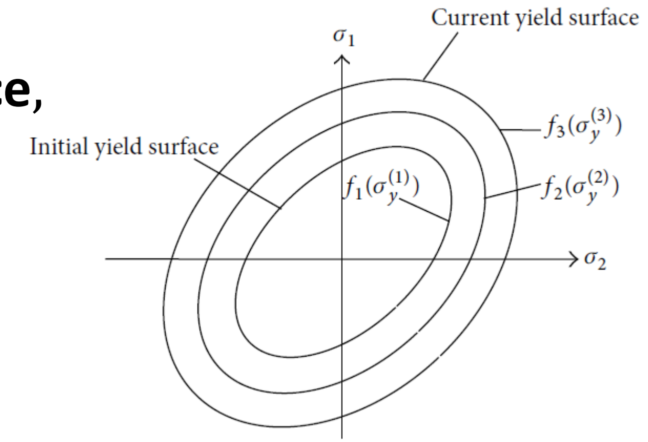


Comparison of melt pool half width and depth between optical measurement and calibrated FEM

Mechanical property requirements

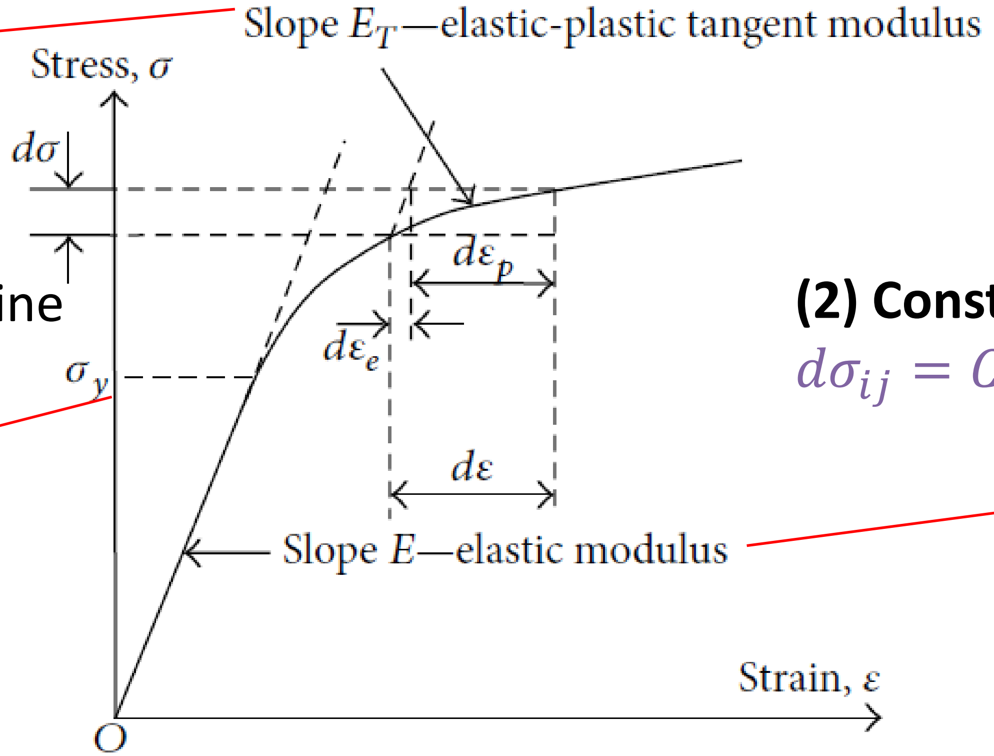
(4) Hardening: Progressive development of yield surface,

$f = \sigma_y(k) \qquad k = \epsilon^p_{eff}$



Isotropic hardening model

$$\frac{d\sigma_{eff}}{d\epsilon^p_{eff}} = \frac{\boldsymbol{E_T}}{1 - \left(\boldsymbol{E_T}/\boldsymbol{E}\right)}$$



(3) Yield criterion (to define plastic flow initiation)

$\sigma_{eff} = \sqrt{3}\boldsymbol{\sigma_y}$

von Mises effective stress

(2) Constitutive relation:

$d\sigma_{ij} = C^e_{ijkl} d\epsilon^e_{kl} + dC^e_{ijkl}\epsilon^e_{kl}$

$C_{ijkl} = f(\boldsymbol{E}, \boldsymbol{\nu})$
(for isotropic materials)

$d\epsilon^e_{kl} = d\epsilon_{kl} - d\epsilon^p_{kl} - d\epsilon^{th\_\alpha}_{kl}$

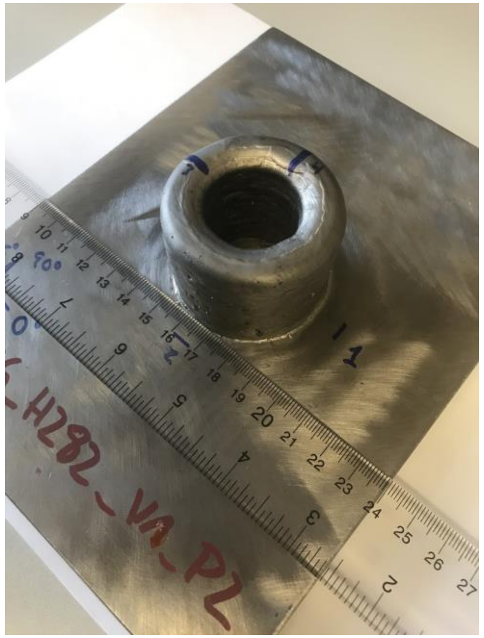
(5) Uniaxial stress-strain curve at different T

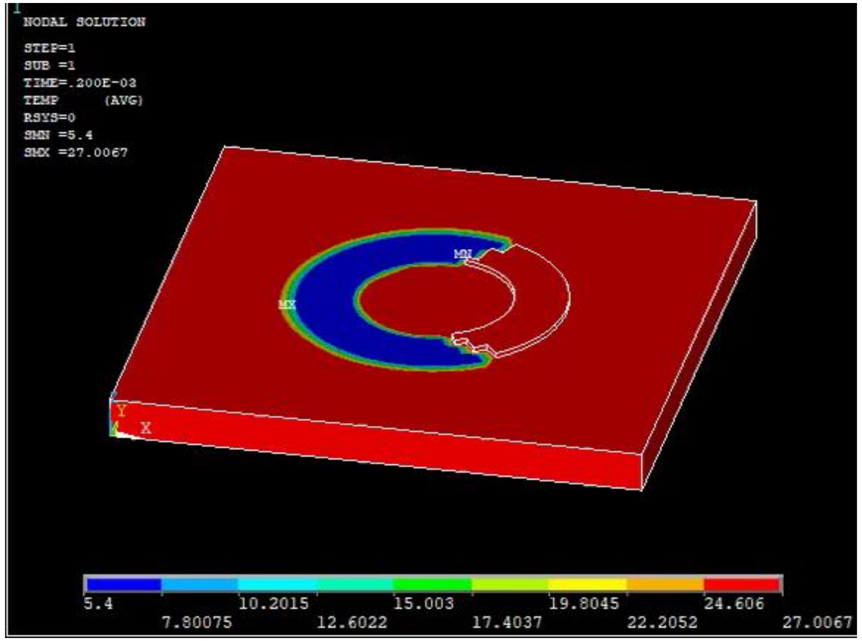
(1) $d\epsilon^{th\_\alpha}_{kl}(T) = \boldsymbol{\alpha}\,(T - T_0)$

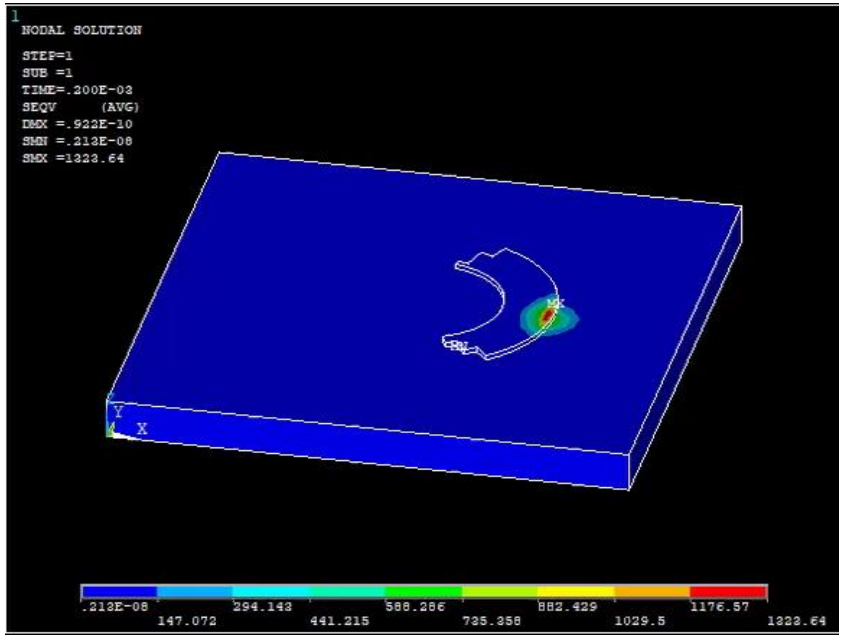
Thermomechanical simulation

Temperature(°C)

Stress, σ_{eff}(Pa)

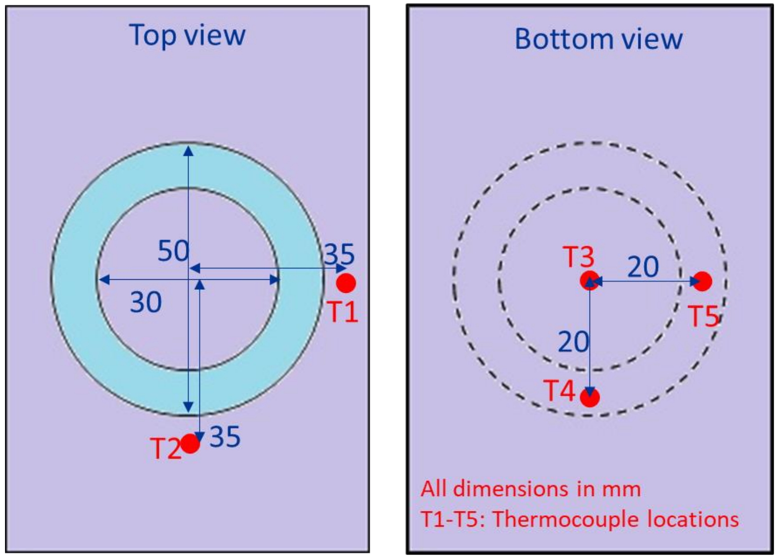


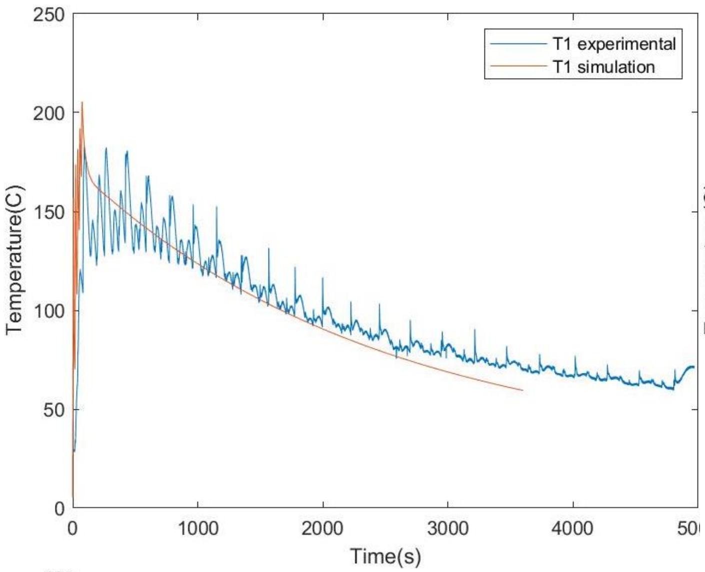


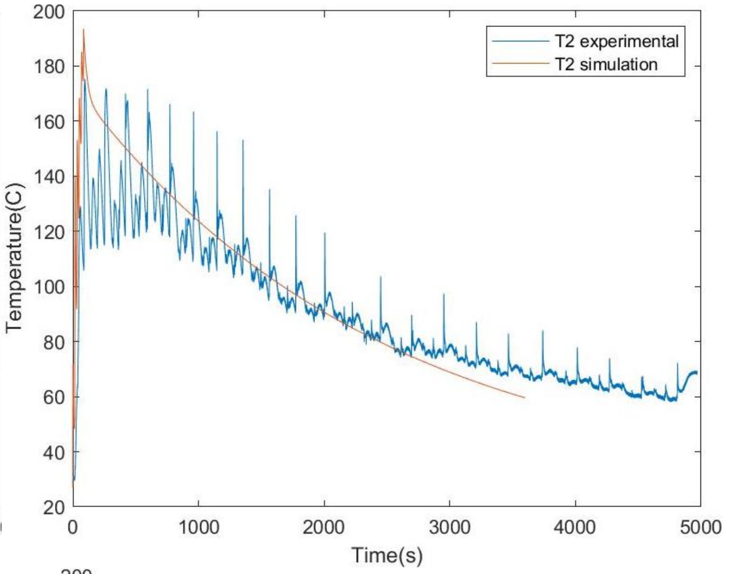


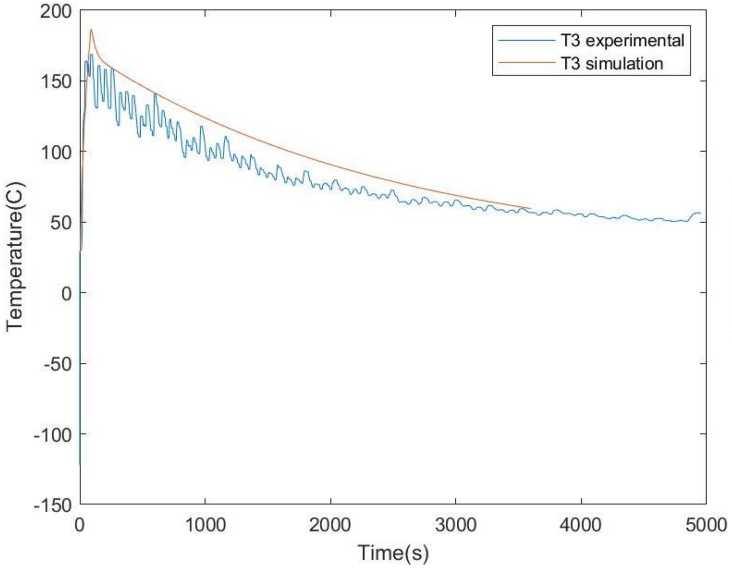
Simulation time ~68 hrs.

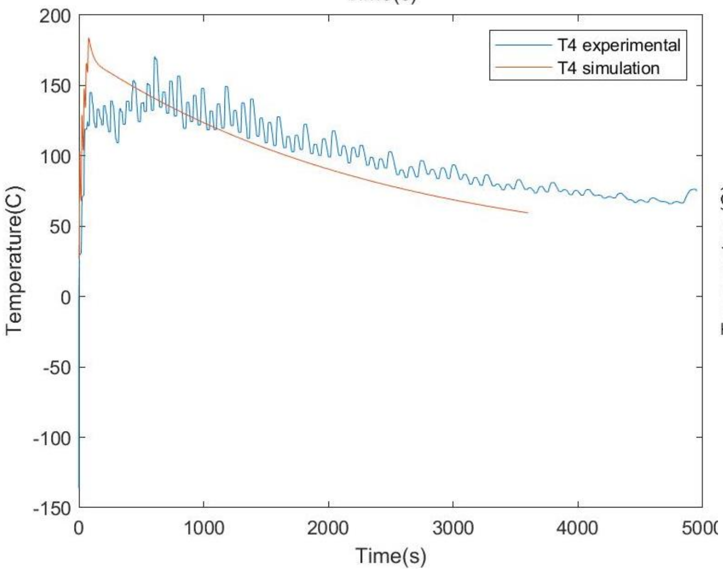
Thermal model calibration: Cylinder

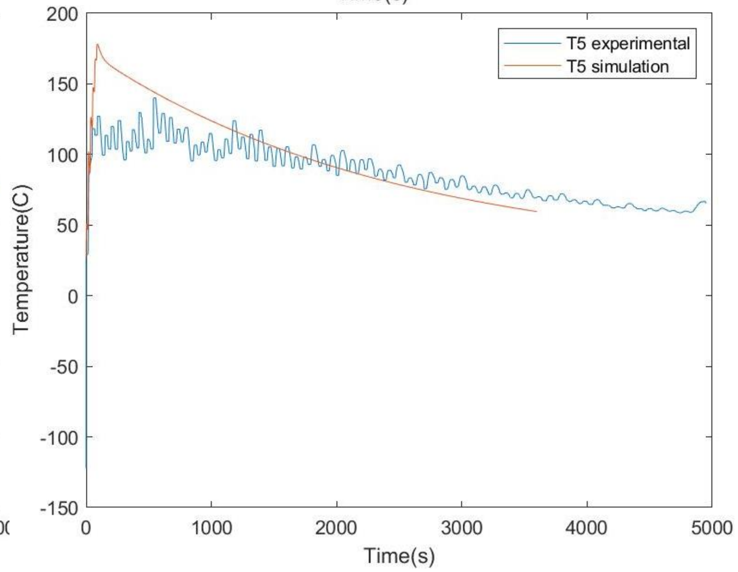






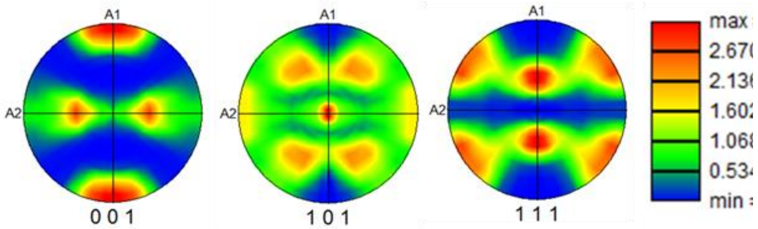






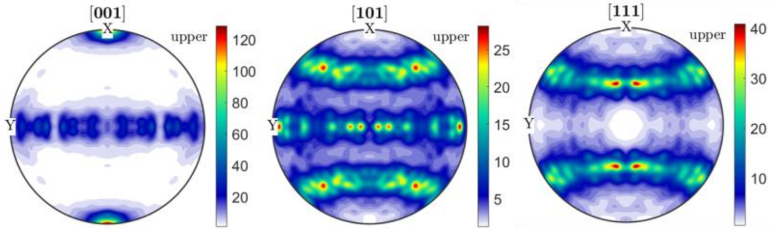
DDD model calibration: Multitrack

EBSD

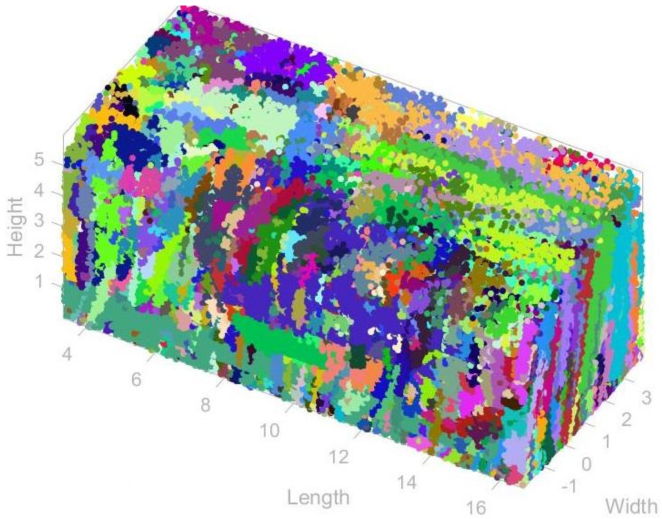


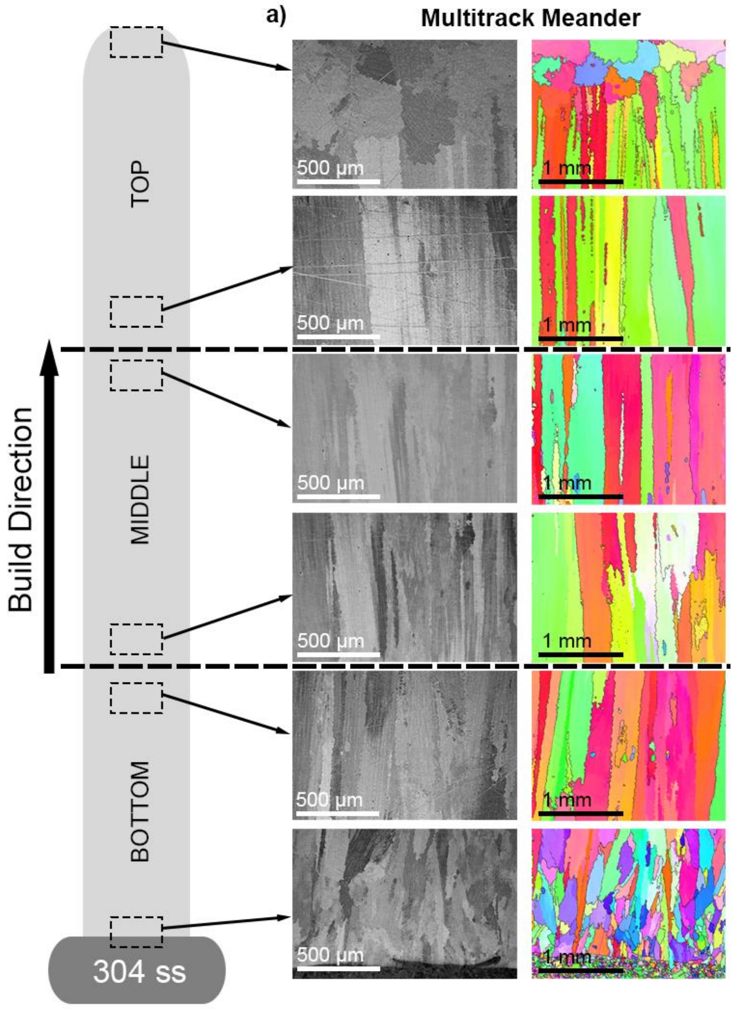
Grain growth simulation using MP dimensions obtained after heat source calibration

Simulation



- Comparing pole figures at different locations
- Cannot simulate entire block. Simulating in parts





Planned studies in this project (next step)

ICME modeling enhanced by machine learning

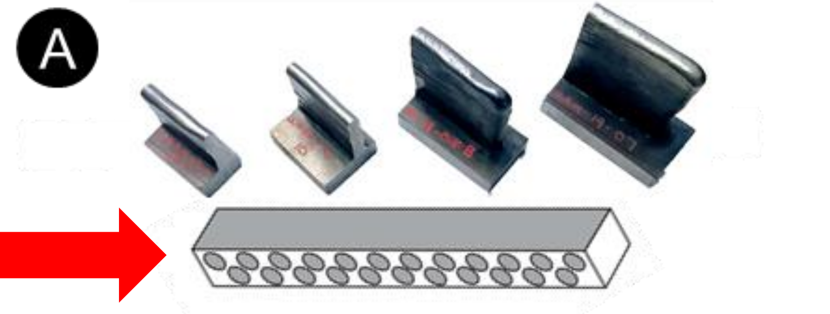
A1. As-print microstructure study on WAAM HAYNES 282

A2. Recrystallization study on WAAM HAYNES 282

A3. HT Aging study on WAAM HAYNES 282

B1. Location specific microstructure respond based on processing parameters (print + heat treatment)

Shape effect:
Height & Cross section

A	B
	 Cone shape
HT WAAM sample with gradient temperature and processing parameter	Complex geometry build for location specific ICME design

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