University of Pittsburgh | Swanson School of Engineering

Department of Mechanical Engineering & Materials Science

2023 FECM Spring R&D Project Review Meeting

DE-FE0026825 (UCFER RFP 2020-06) The University Coalition for Fossil Energy Research

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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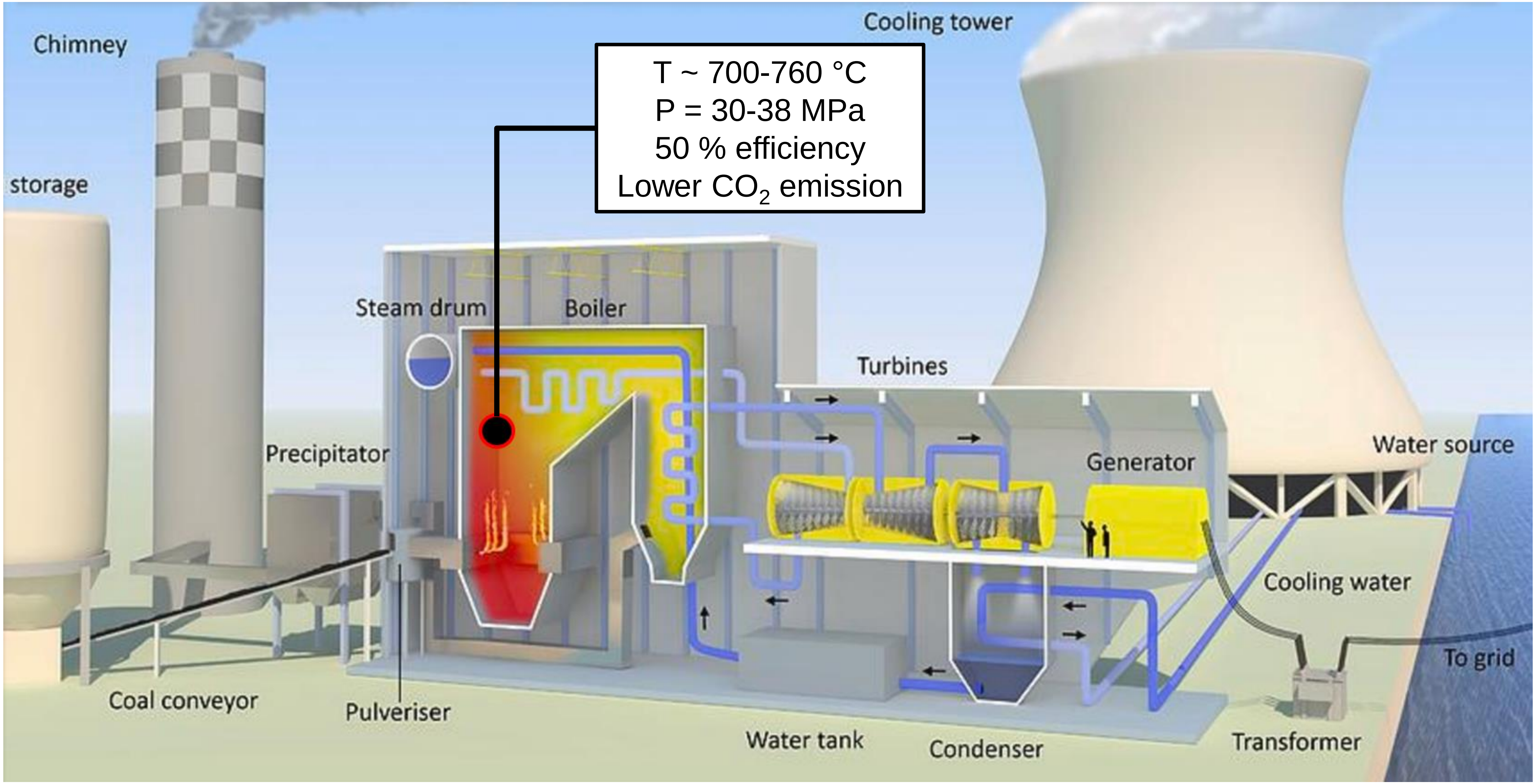
Oliver Hermann, Daniel Kuehne, Alexander Riemann, Andrea Clark (Gefertec)

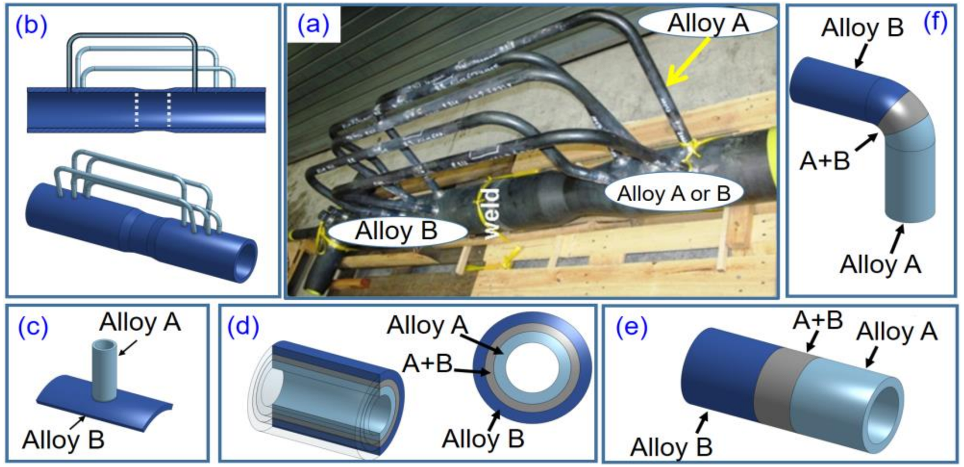
NATIONAL ENERGY TECHNOLOGY LABORATORY | PennState | SIEMENS energy | GEFERTEC | HAYNES International | University of Pittsburgh

Motivation: A-USC Coal Power Plants Eco-Efficiency

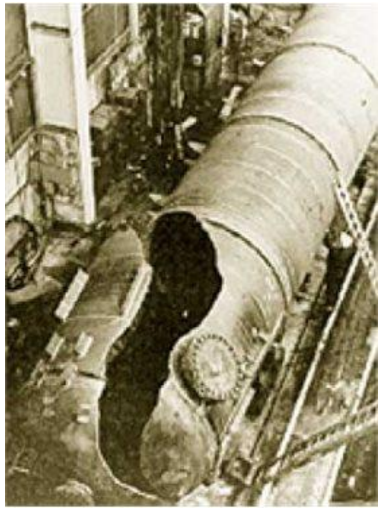


Motivation: Repair and join

Complex shape manufacturing



Repair pipeline in a rapid mode

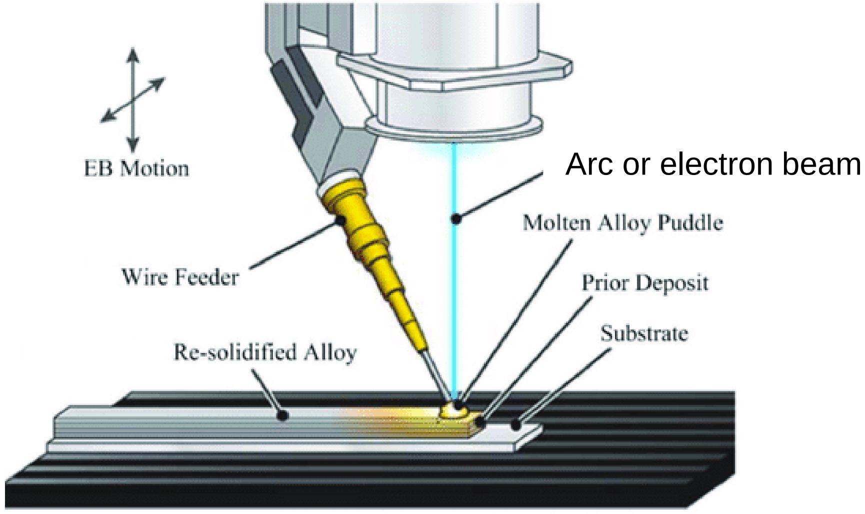


Images from internet

Images from internet

Motivation: WAAM

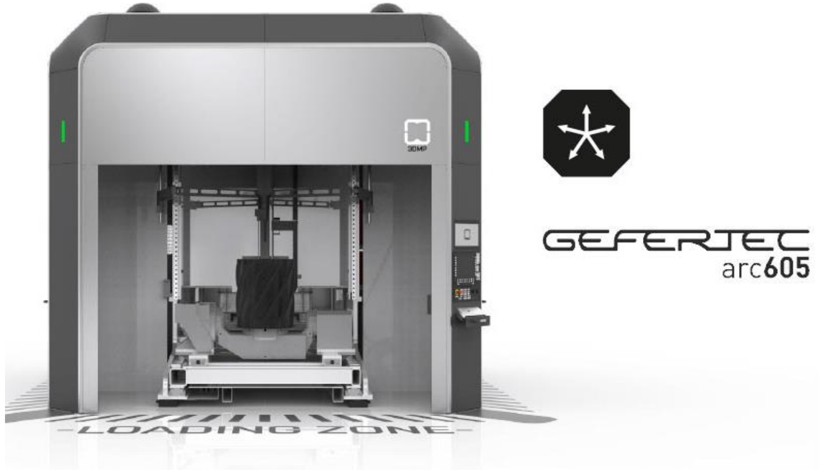
Wire-arc additive manufacturing (WAAM)



DOI: 10.3390/en15031076

- Low running cost and short production cycle
- high deposition rates
- minimum wastage of materials
- Ability to build large parts
- Main disadvantage is
  - lower precision in as-built parts

Directed Energy Deposition



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

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

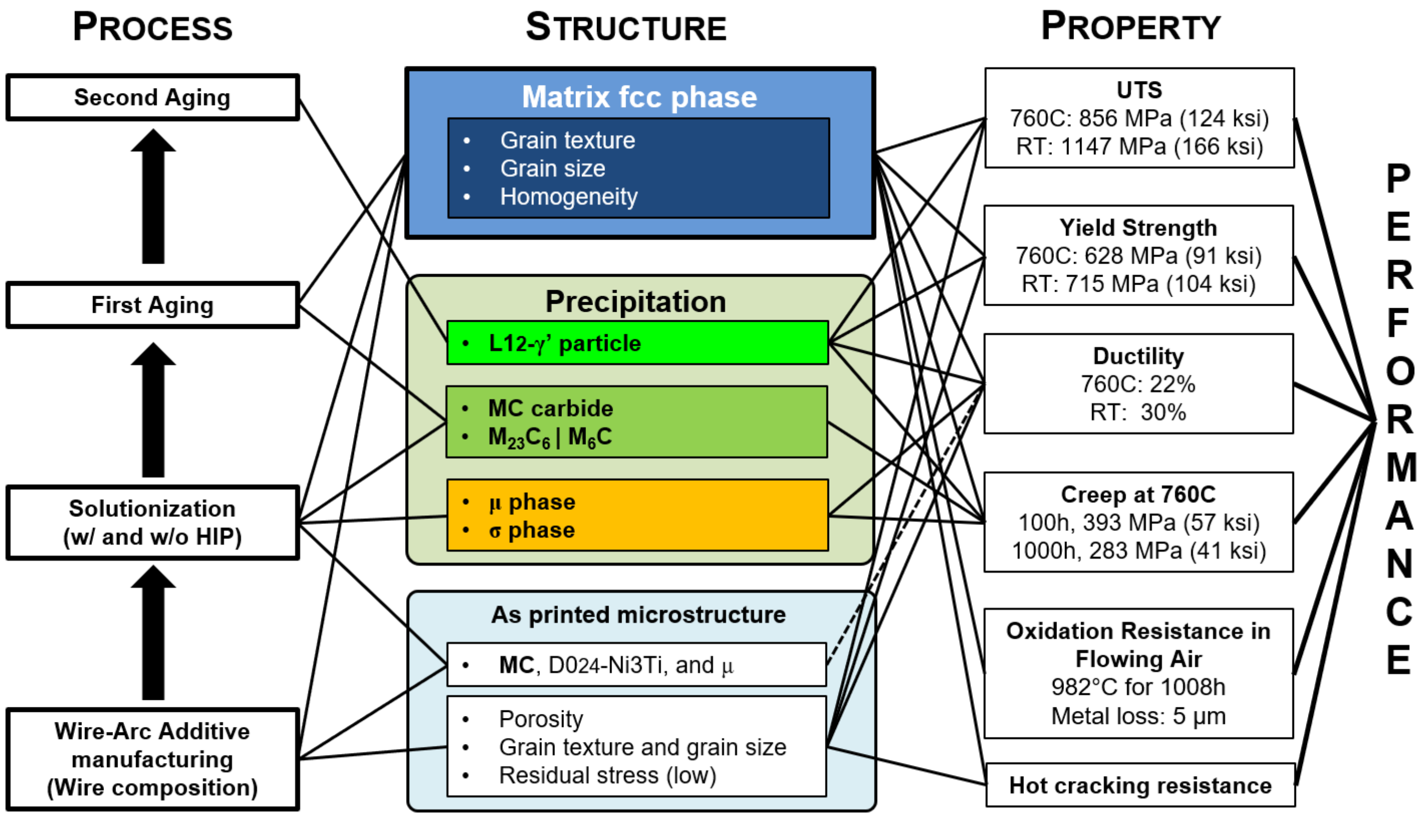
WAAM process | Post-heat treatment

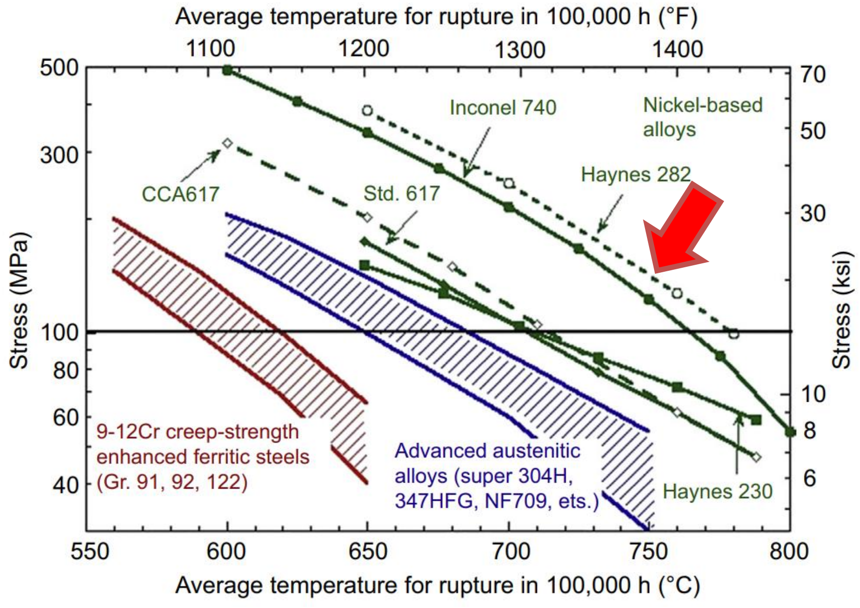
Design Solutions using the Extended ICME Platform at Pitt

(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, NATIONAL ENERGY TECHNOLOGY LABORATORY, SIEMENS energy, GEFERTEC, PITT MOST-AM

Haynes 282®: Systems Design Chart



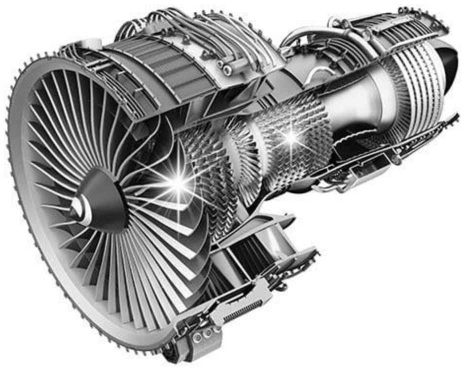


DOI: 10.1016/B978-0-08-100552-1.00015-4

Haynes 282®: Microstructure

Chemical Resistance
- Oxidation
- Corrosion

Mechanical Resistance
- Traction
- Fracture
- Impact
- Creep



Primary TiN and Ti, Mo-rich MC phases

Secondary/Primary Mo-Ni rich M_6C and Cr, Mo-rich $M_{23}C_6$ carbides

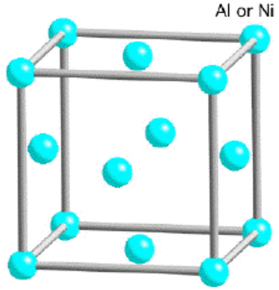
$$MC + \gamma \rightarrow M_{23}C_6 + \gamma'$$

$$(Ti, Mo)C + (Ni, Cr, Al, Ti) \rightarrow Cr_{21}Mo_2C_6 + Ni_3(Al, Ti)$$

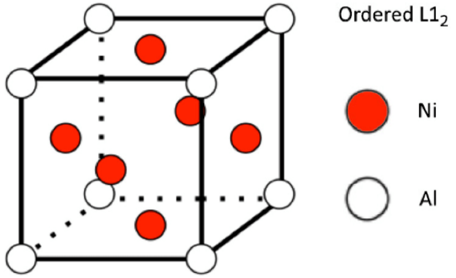
$$MC + \gamma \rightarrow M_6C + \gamma'$$

$$(Ti, Mo)C + (Ni, Cr, Al, Ti) \rightarrow Mo_3(Ni, Co)_3C_3 + Ni_3(Al, Ti)$$

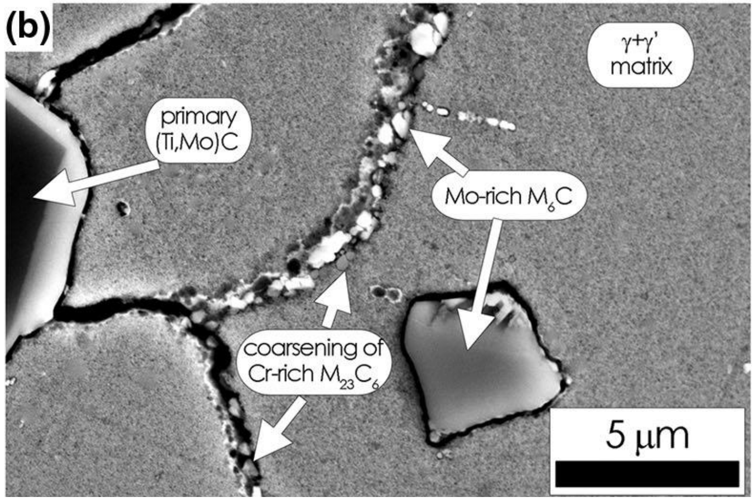
γ phase , fcc



γ' phase (L12),$Ni_3(Al, Ti)$

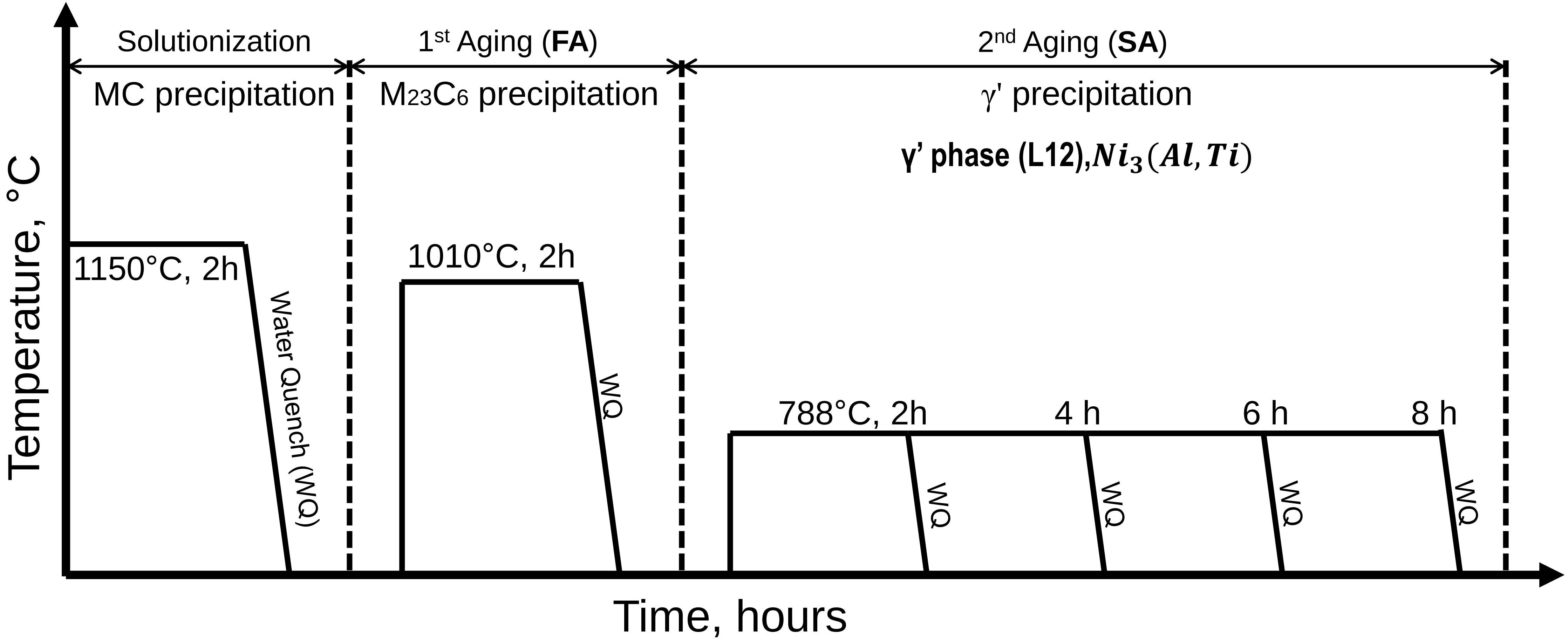


$$k_{Co}^{Ni} = 1, k_{Cr}^{In718} = 1.03, k_{Al}^{In718} = 1, k_{Ti}^{In718} = 0.69, k_{Mo}^{In718} = 0.82$$



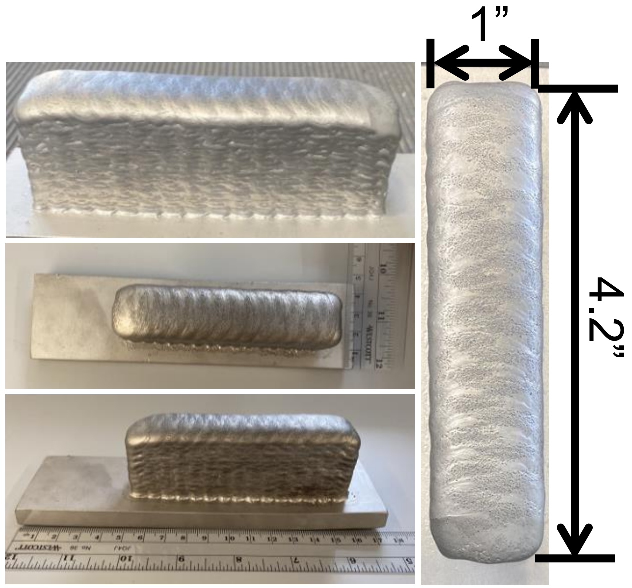
Y. Yang, MICROSTRUCTURAL EVOLUTION IN CAST HAYNES 282 FOR APPLICATION IN ADVANCED POWER PLANTS.
A. Ramakrishnan, Microstructure and mechanical properties of direct laser metal deposited Haynes 282 superalloy, 2019

Haynes 282®: Heat treatment

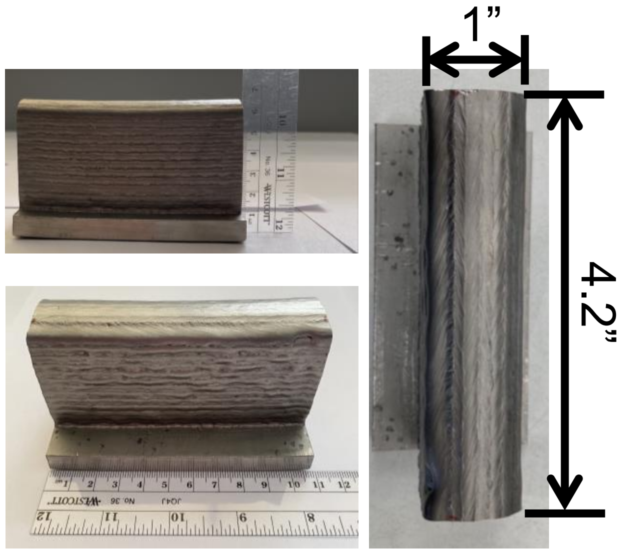


- The effect of solution temperature and aging time on gamma prime precipitation was systematically studied.
- FA and SA mean first and second aging, respectively.

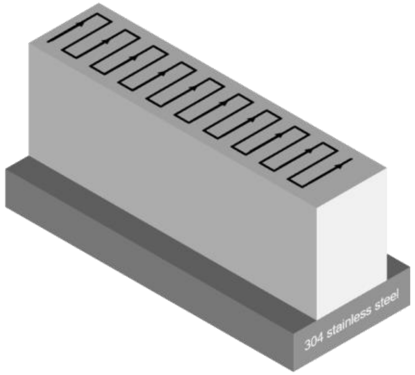
Printing strategy difference: Meander vs. Single Bead



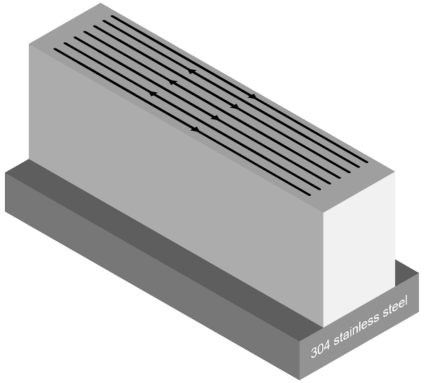
Multitrack Meander Haynes 282



Multitrack Single Bead Haynes 282



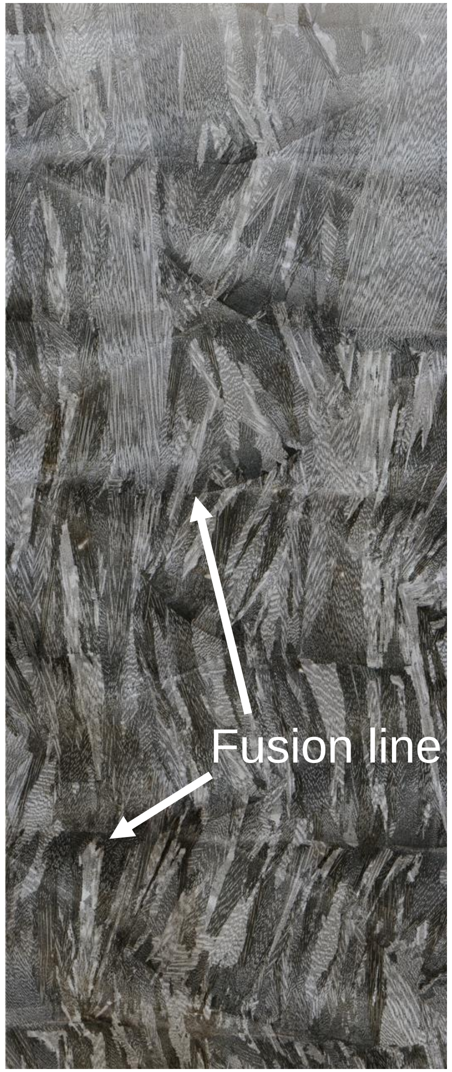
Zigzag, Meander



Single bead

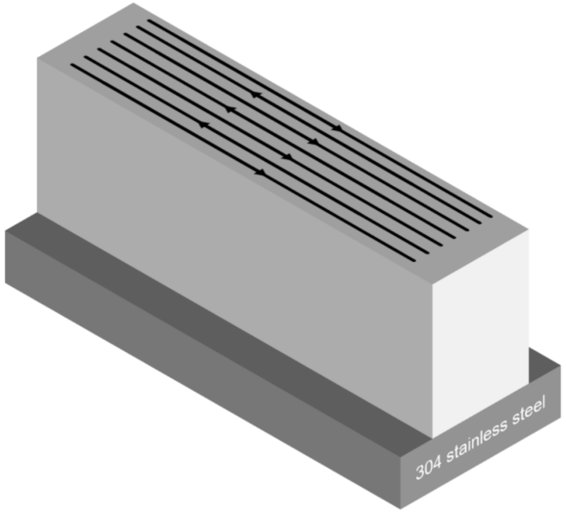
As-printed grain structure: Single Bead vs. Meander

Build direction, Z

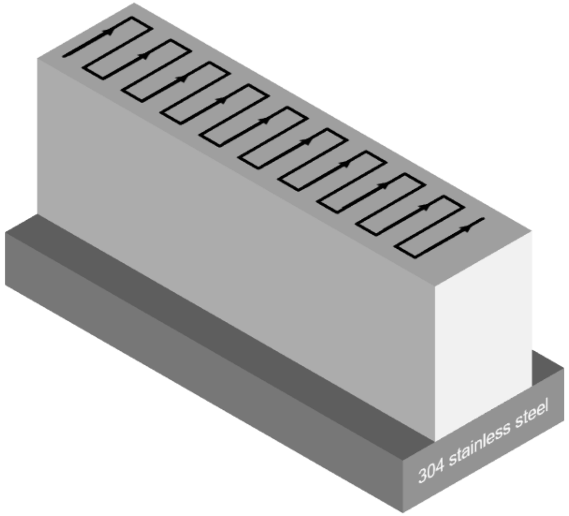


5 mm

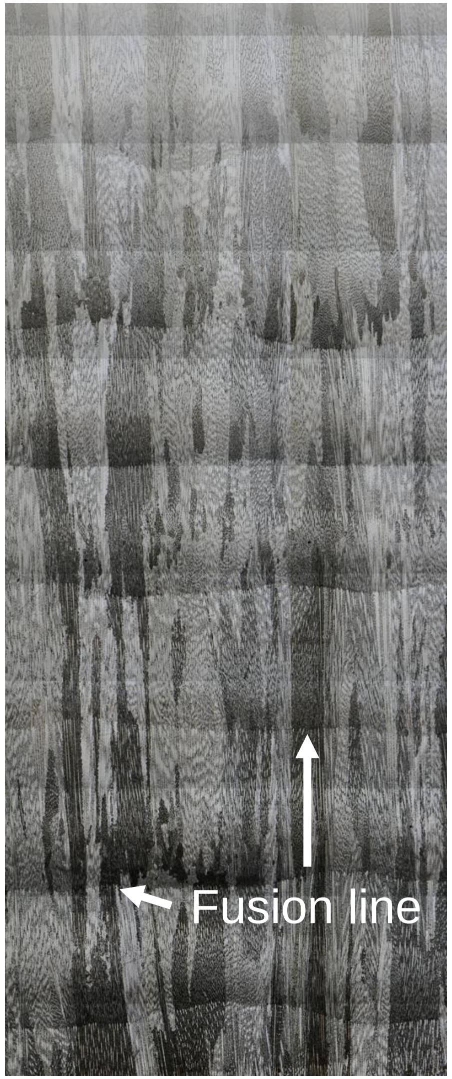
Single bead



vs.



Zig-zag (meander)

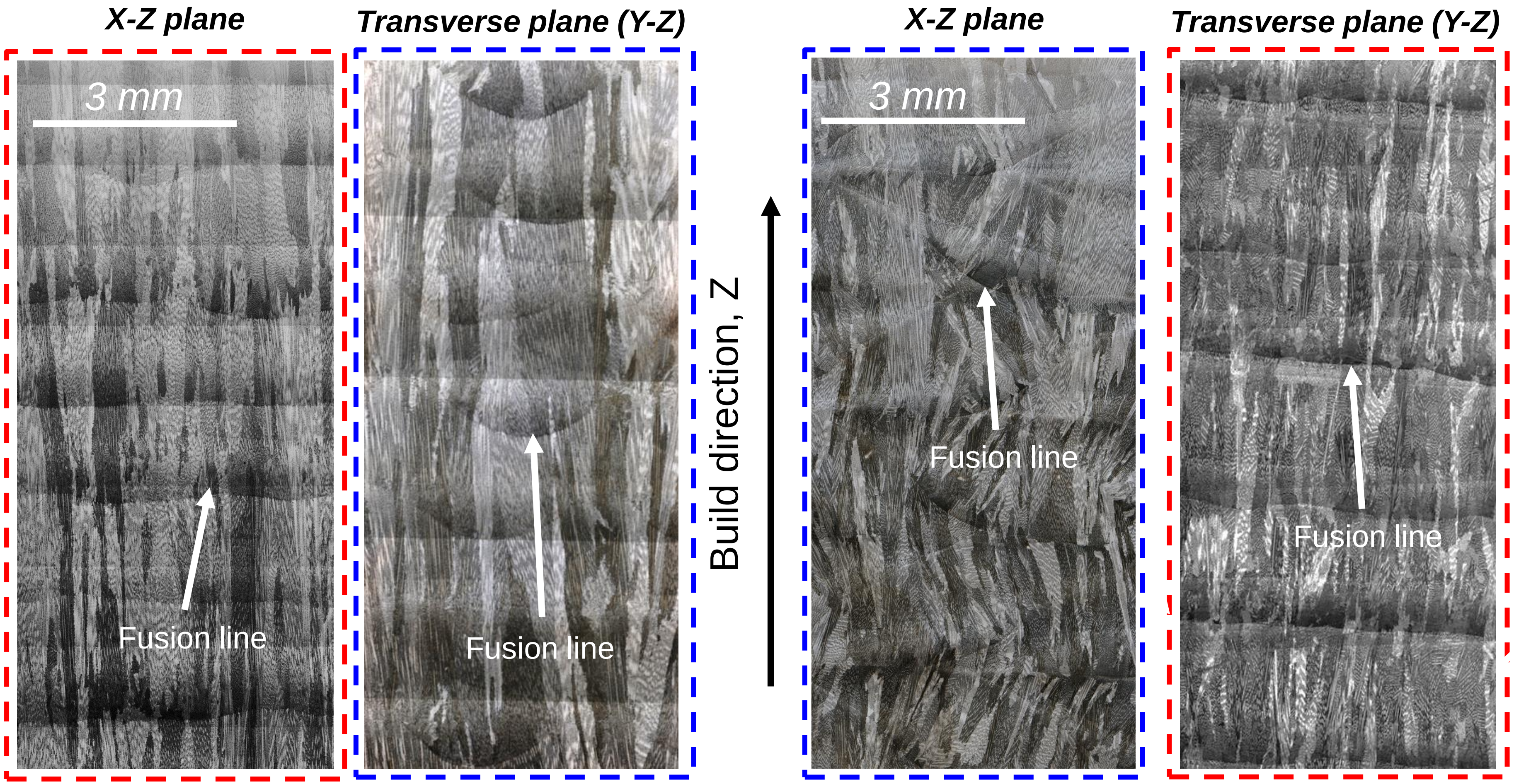


5 mm

As-printed microstructure: Meander vs. Single Bead

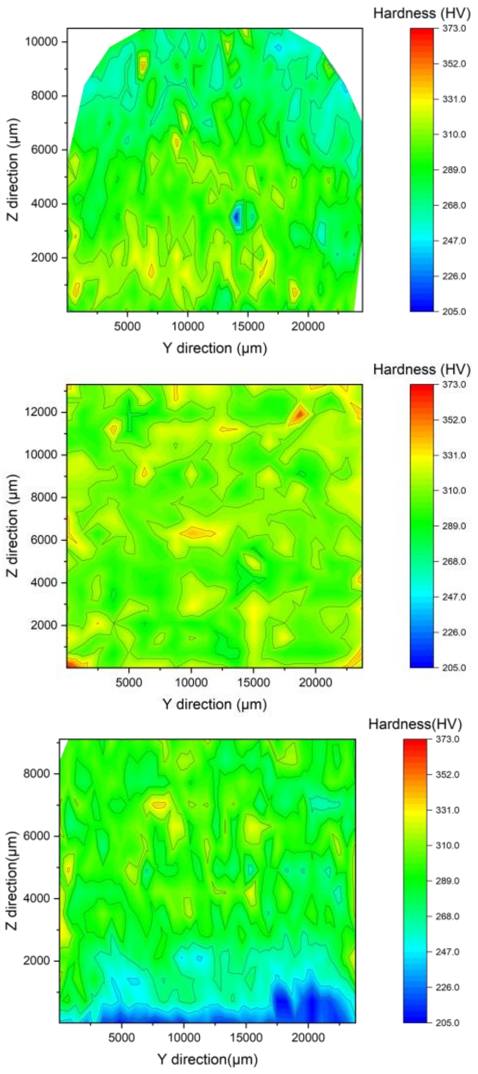
Similarities can be found between **X-Z plane of Meander** and **Y-Z (transverse) plane of Single bead**
Y-Z (transverse) plane of Meander and **X-Z plane of Single bead**

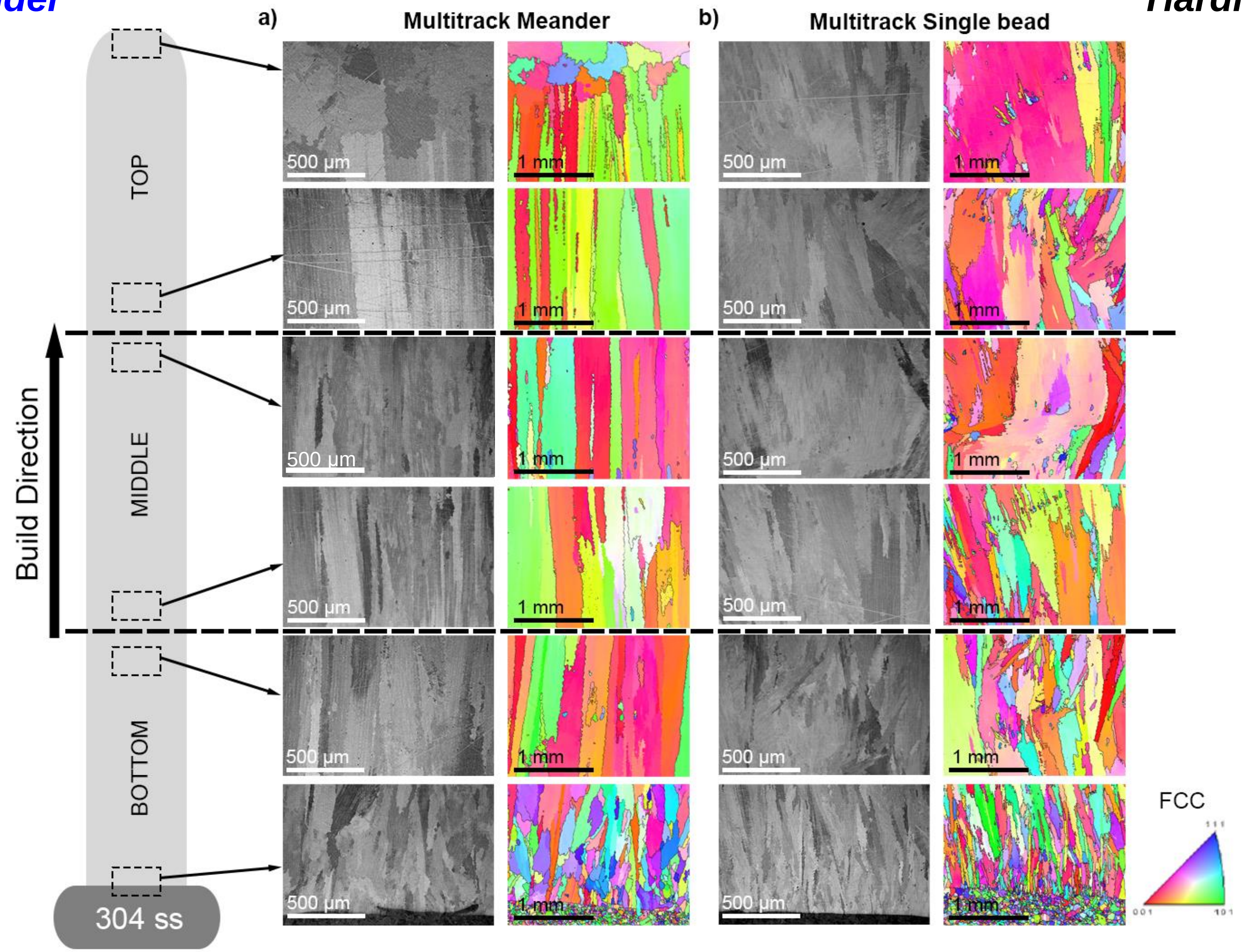
Multitrack **Meander** — Multitrack **Single Bead**



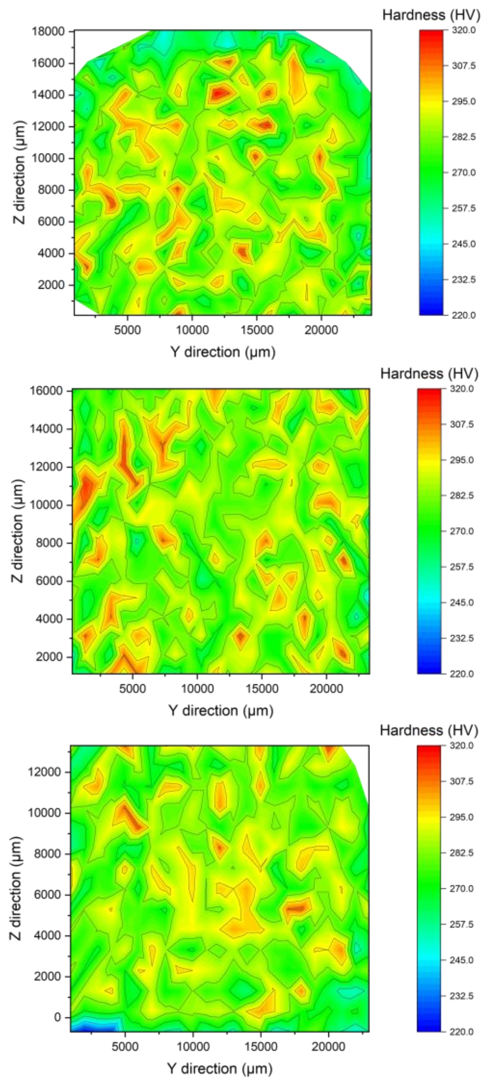
As-printed microstructure: Meander vs. Single Bead

Hardness Map of Meander

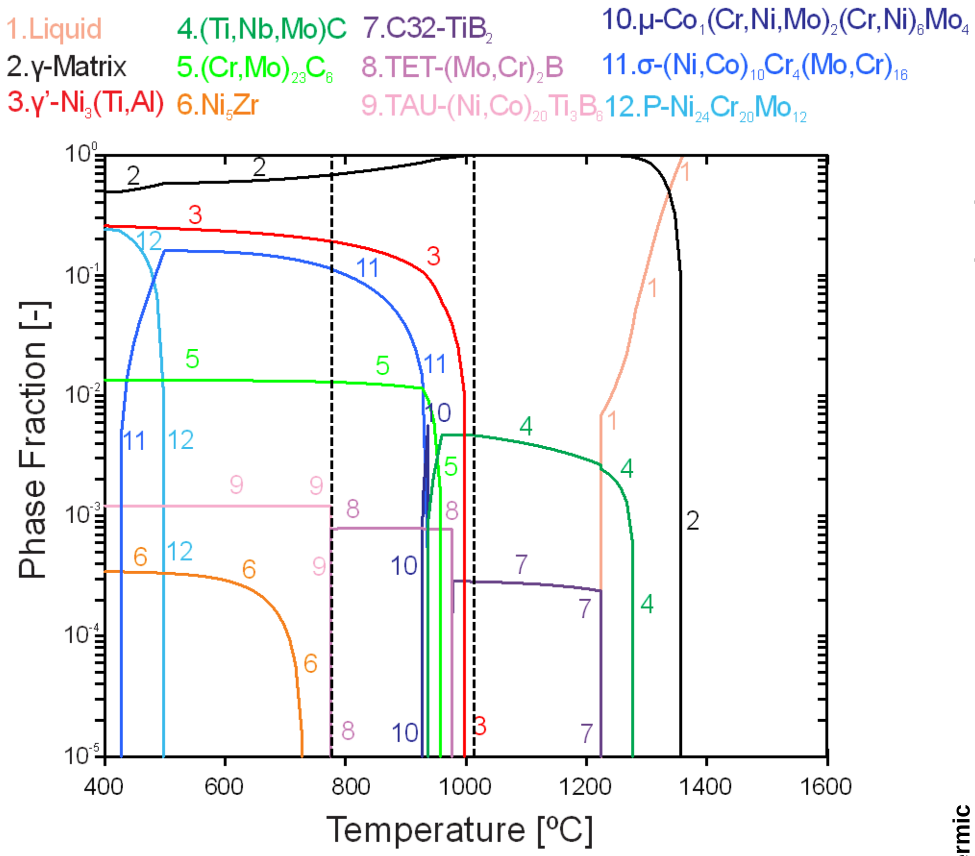




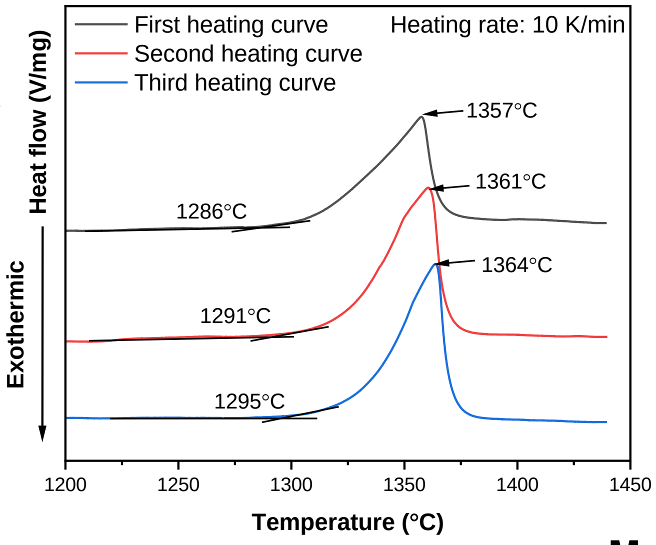
Hardness Map of Single Bead

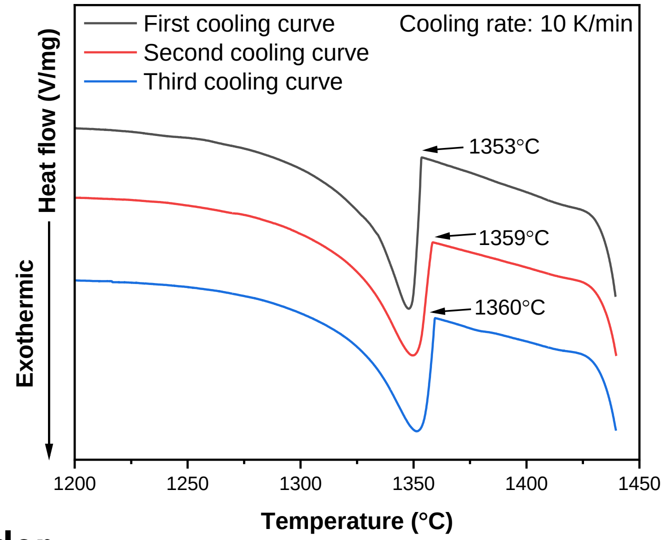


Determination of phase transformation temperature

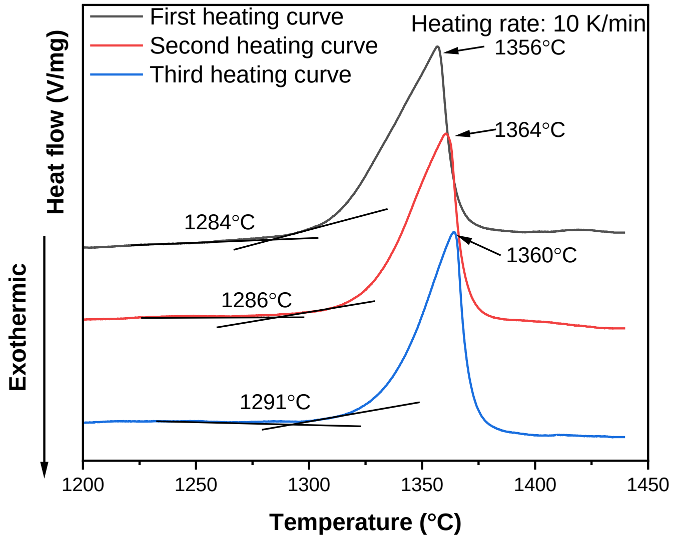


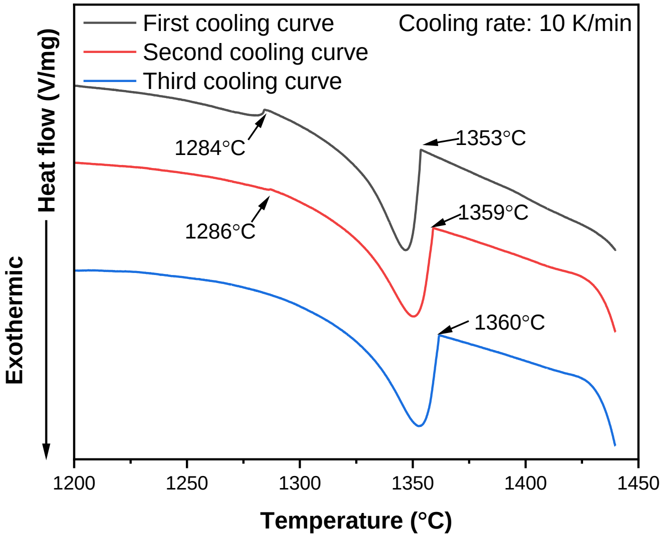
Single-Bead





Meander

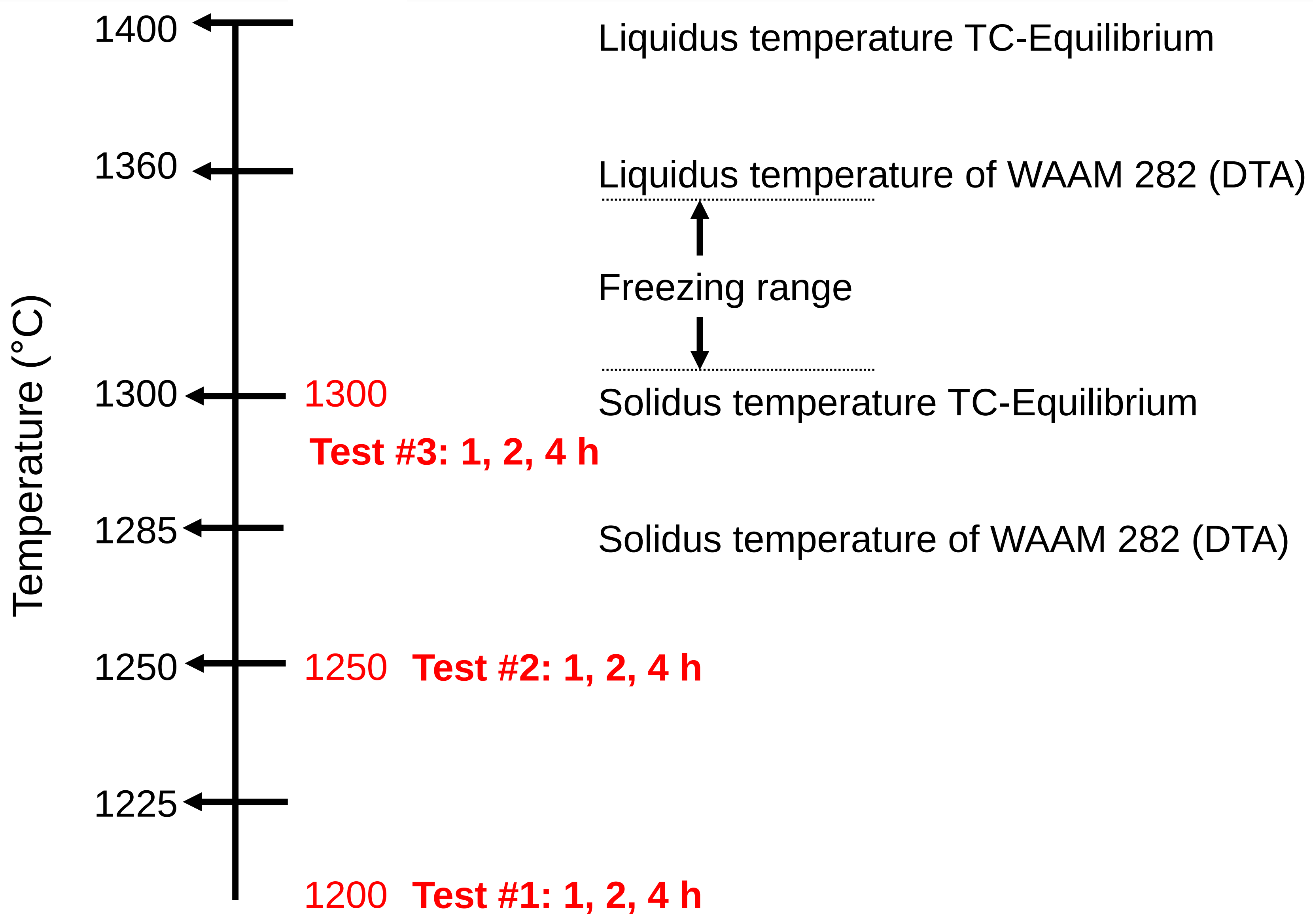




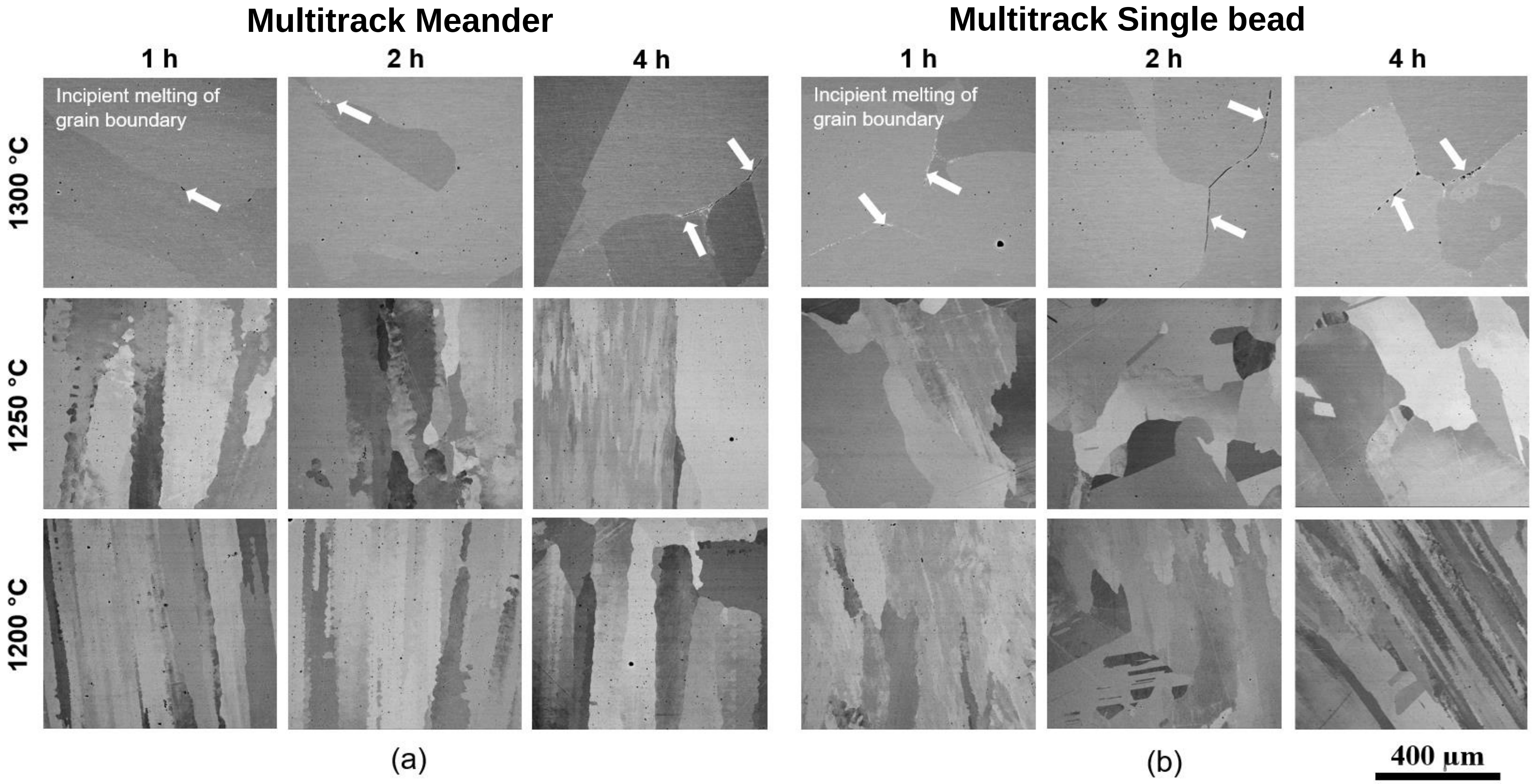
Determination of phase transformation temperature (cont'd)

Transformation temperature	CALPHAD prediction	Meander		Single bead	
		Heating (10 K/min)	Cooling (10 K/min)	Heating (10 K/min)	Cooling (10 K/min)
Solidus	1300 °C	1287.4 ± 3.6	1285.0 ± 1.4	1290.7 ± 4.5	NA
Liquidus	1400°C	1360.0 ± 4.0	1358.0 ± 4.6	1360.7 ± 3.5	1357.3 ± 3.8

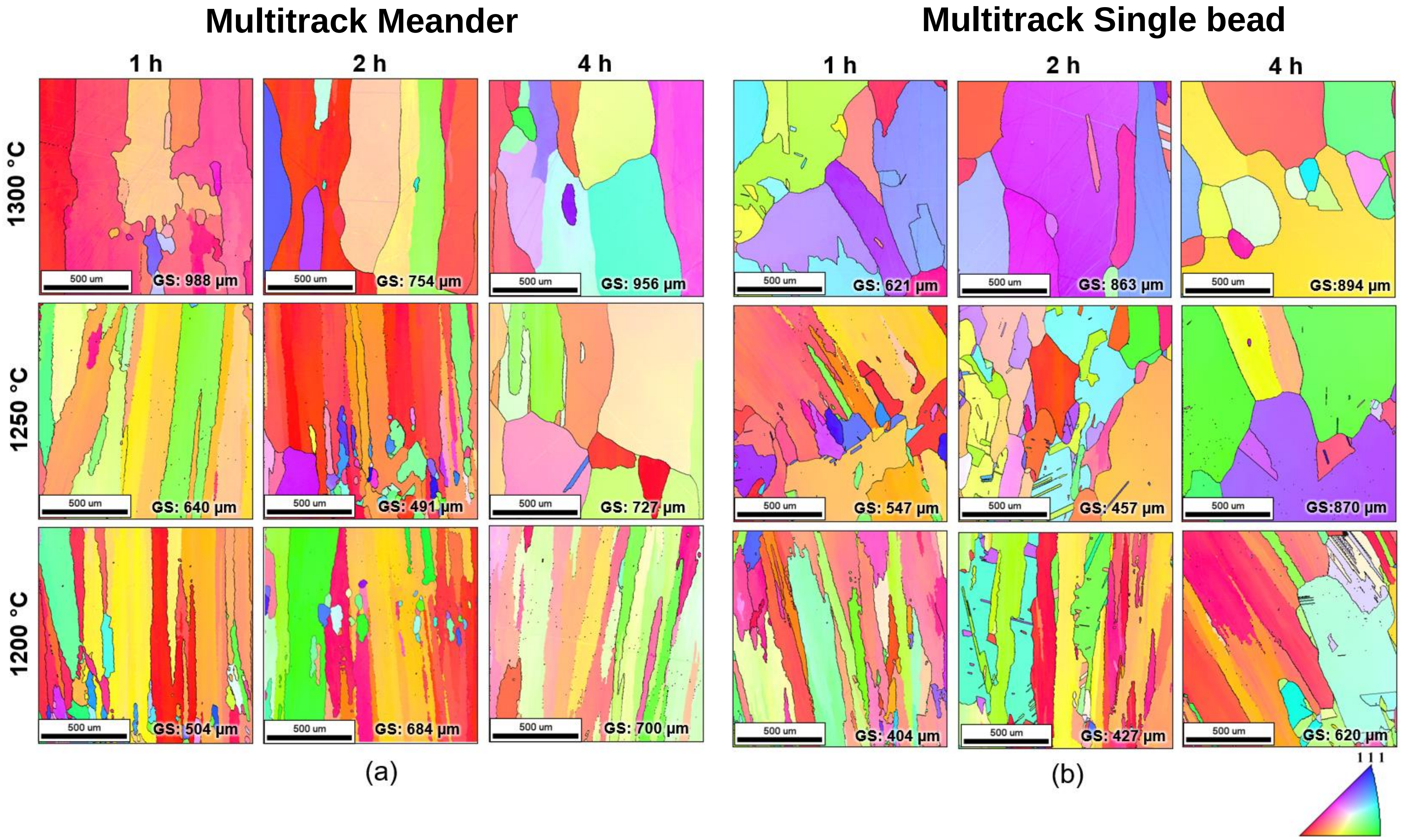
Recrystallization Study: Choice of temperatures



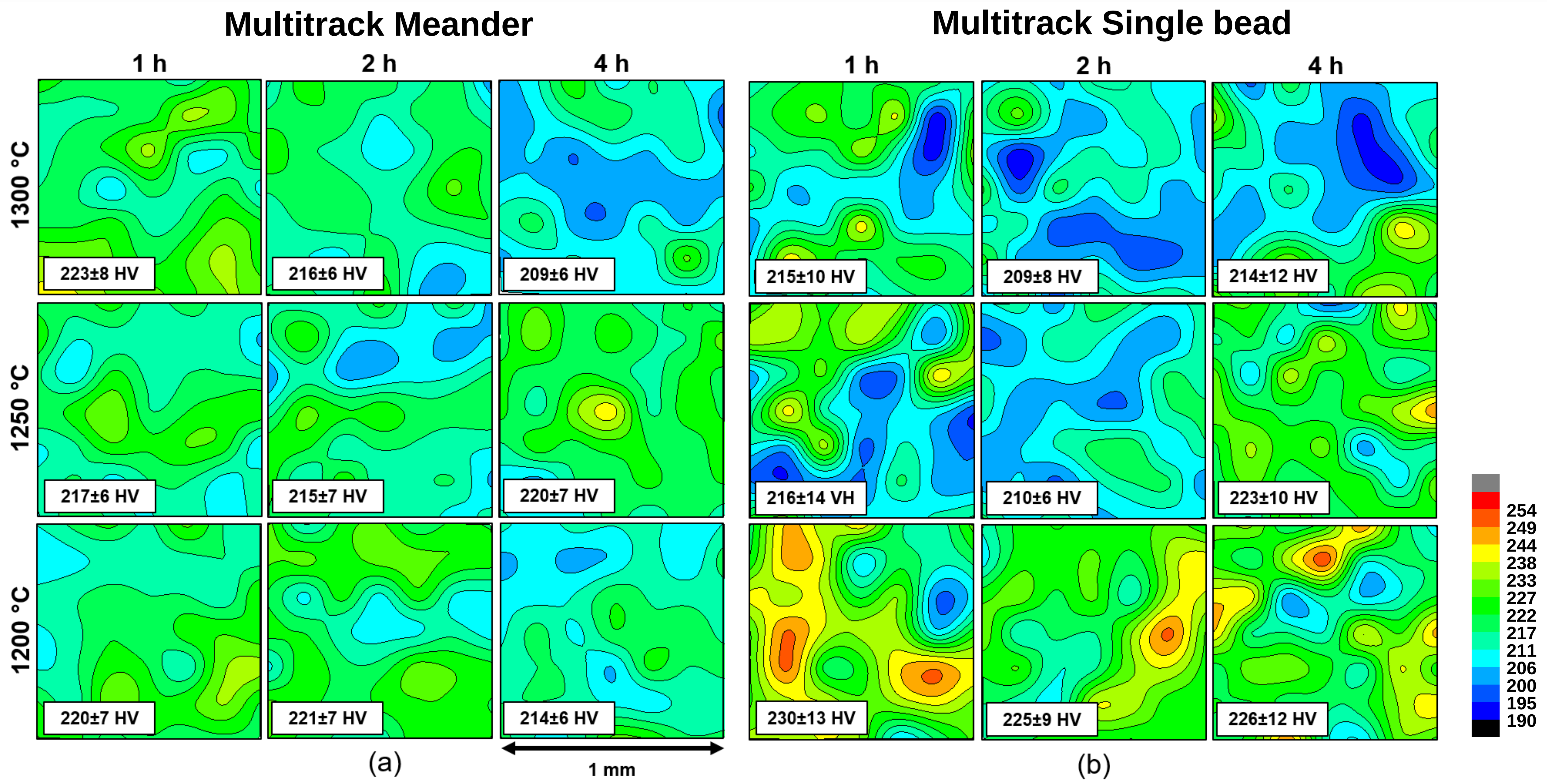
Recrystallization studies for build: **SEM / BSE**



Recrystallization studies for build: **IPF – EBSD**



Recrystallization studies for build: **Hardness**



Summary of recrystallization studies

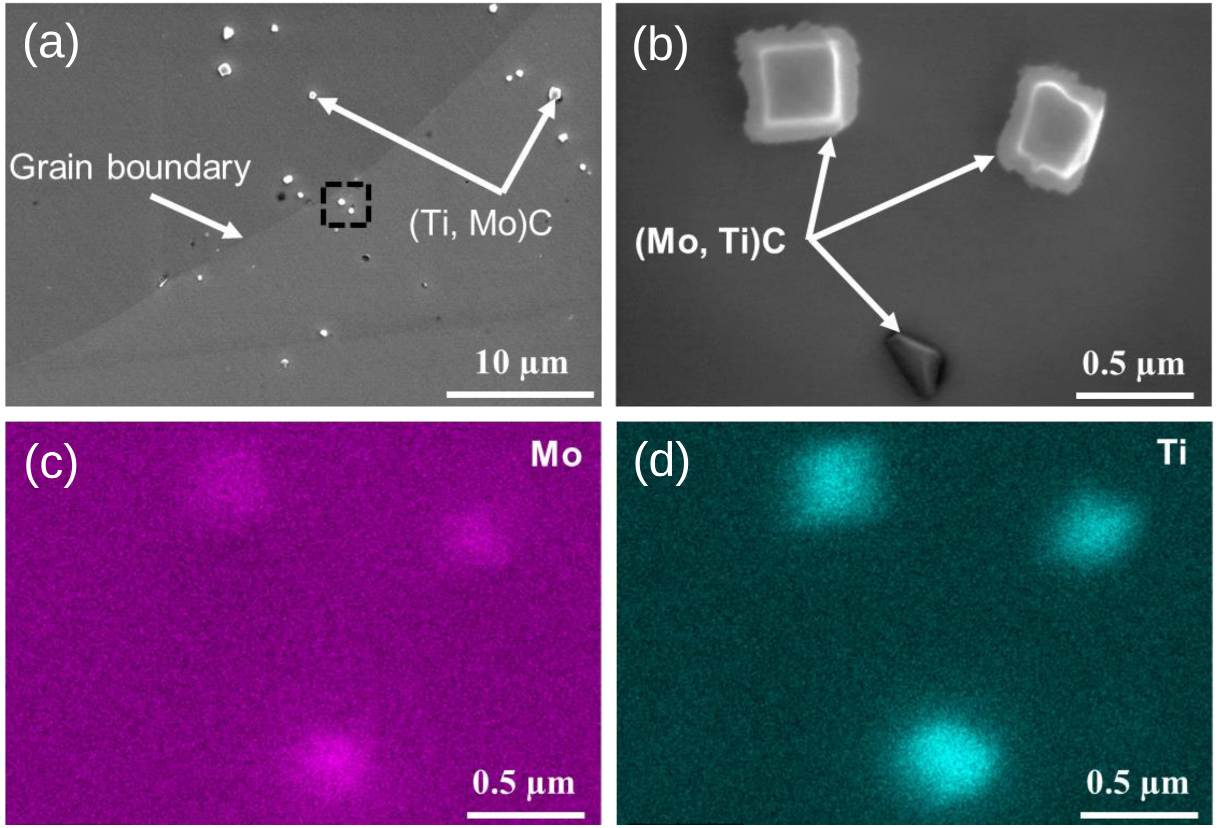
No.	Temperature [°C]	Time [h]	Single Bead		Meander	
			HV_{300g}	Std Dev	HV_{300g}	Std Dev
1	1200	1	230	12.2	220	6.8
2	1200	2	225	8.75	221	6.96
3	1200	4	226	12.14	214	5.64
4	1250	1	216	13.9	217	6.26
5	**1250**	**2**	**210**	**6.33**	**215**	**7.08**
6	1250	4	223	9.91	220	6.71
7	1300	1	215	9.91	223	8.03
8	1300	2	209	7.98	216	5.87
9	1300	4	214	11.69	209	6.28

Optimum

Single bead sample after solution heat treatment at 1250°C for 2 hours

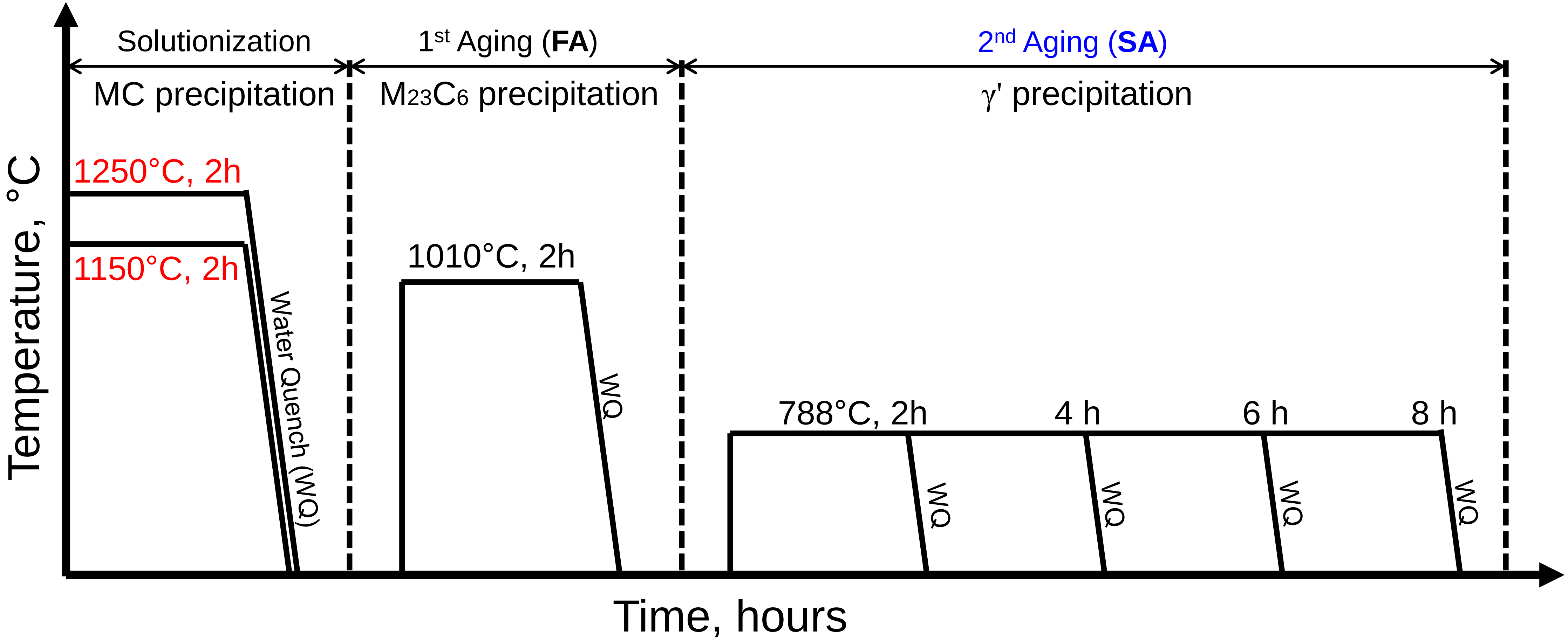
Only MC carbides were observed under this condition.

Single bead
1250°C/2h



- The study on γ' precipitation was carried out on **single bead samples**.
- After a solution treatment at 1250°C for 2 hours, the single bead sample lacks reinforcing phases, γ' and $M_{23}C_6$ carbides.

Effect of solution heat treatment on γ’ precipitation



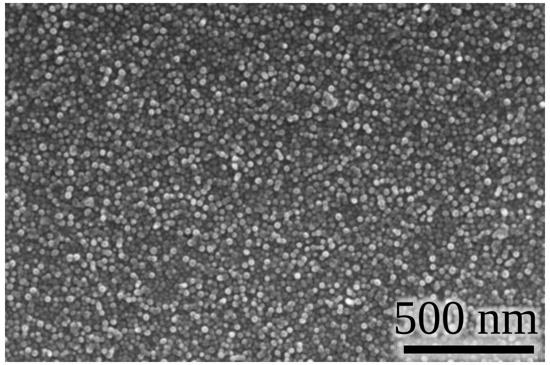
- The effect of solution temperature and aging time on gamma prime precipitation was systematically studied.
- FA and SA mean first and second aging, respectively.

Effect of solution heat treatment on γ' precipitation

ST: Solution Treatment, 2hr
FA: First Aging, 2hr @ 1010°C
SA: Second Aging, @788°C

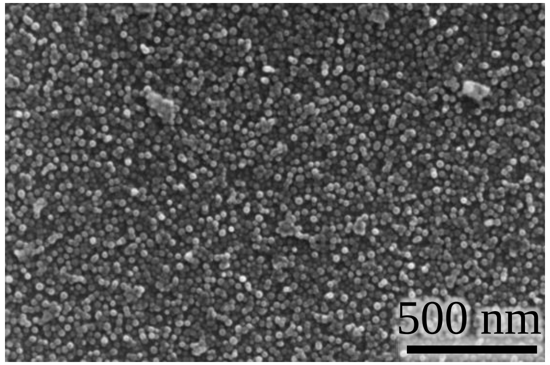
(a) **1250-FA-SA *x*h**

2h



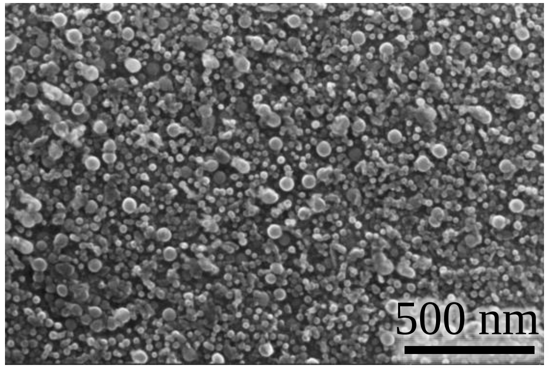
20.32 ± 3.08 nm

4h



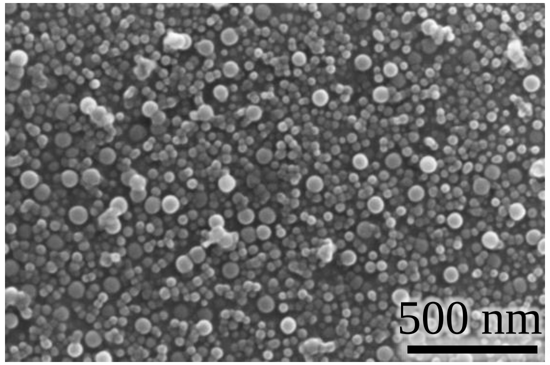
22.73 ± 4.62 nm

6h



25.59 ± 4.60 nm

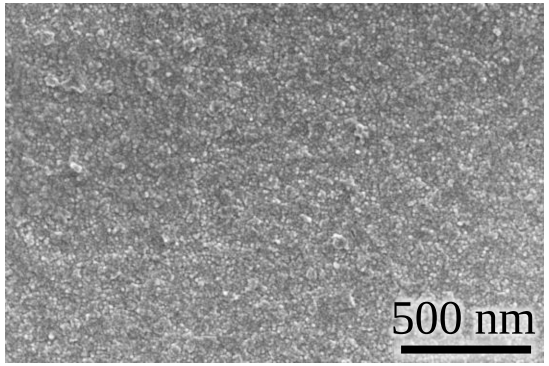
8h



30.73 ± 7.36 nm

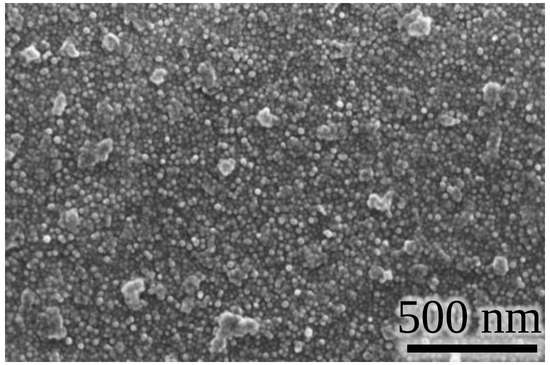
(b) **1150-FA-SA *x*h**

2h



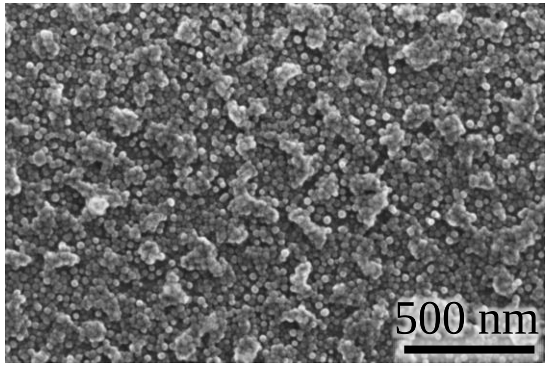
12.95 ± 1.34 nm

4h



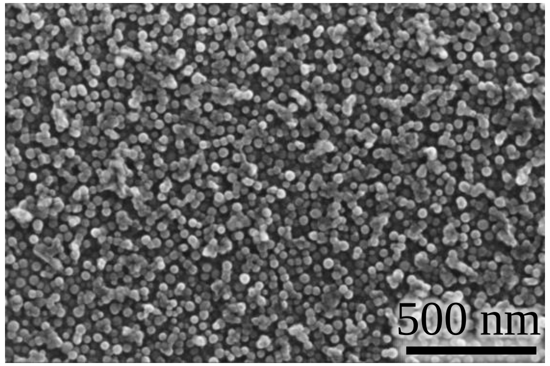
17.92 ± 4.01 nm

6h



25.42 ± 2.04 nm

8h



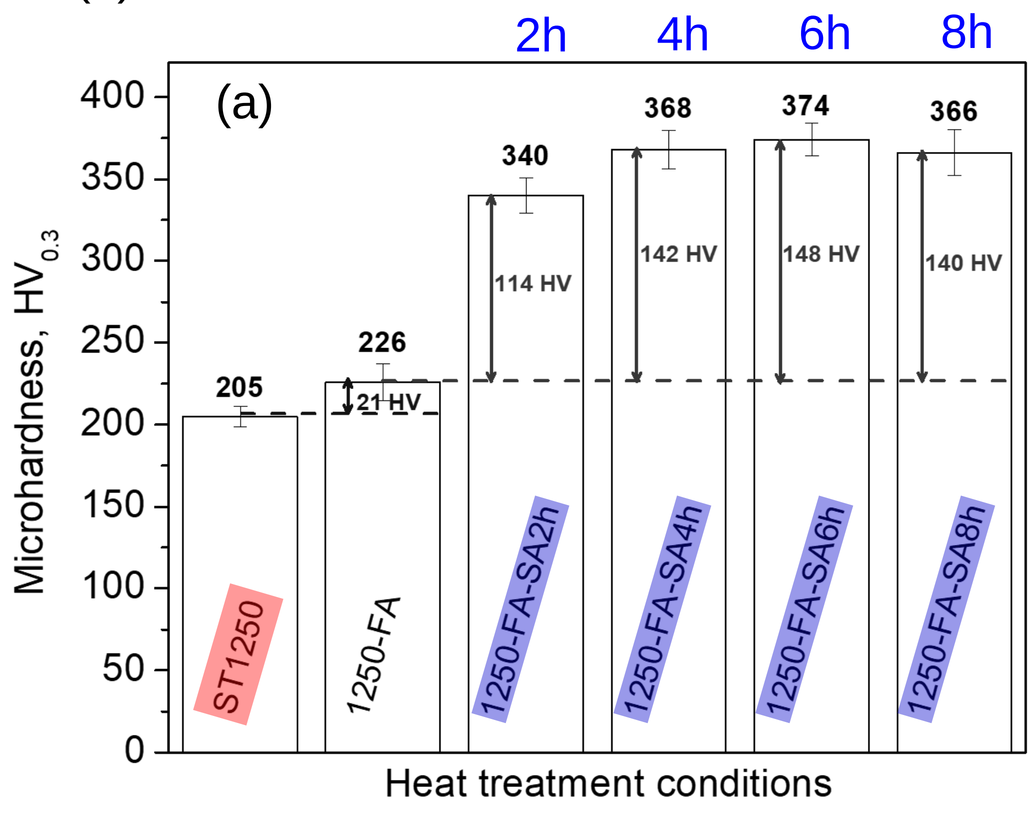
28.19 ± 2.73 nm

Hardness evolution

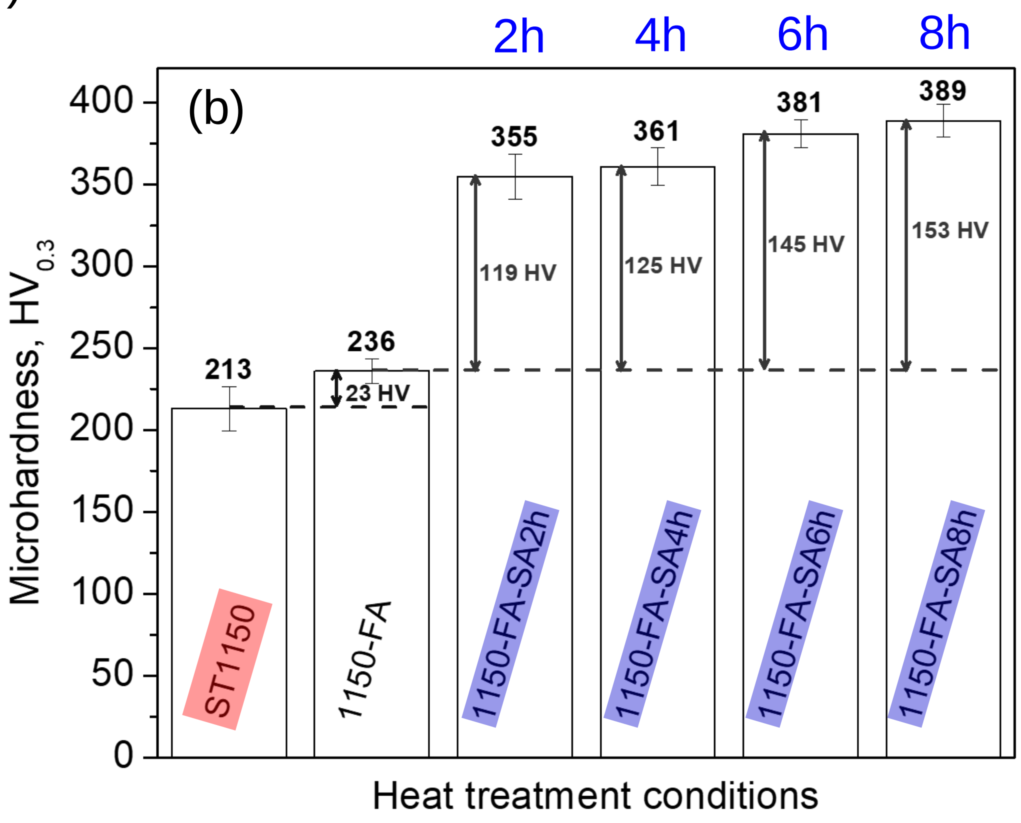
ST: Solution Treatment, 2hr
FA: First Aging, 2hr @ 1010°C
SA: Second Aging, @788°C

- The hardness peak is achieved slightly faster in samples exposed to 1250°C during solution heat treatment.
- The hardness of samples 1150-FA-SA8h and 1250-FA-SA6h show a hardness **similar to** the hardness of Haynes 282 made by forging (373 HV)

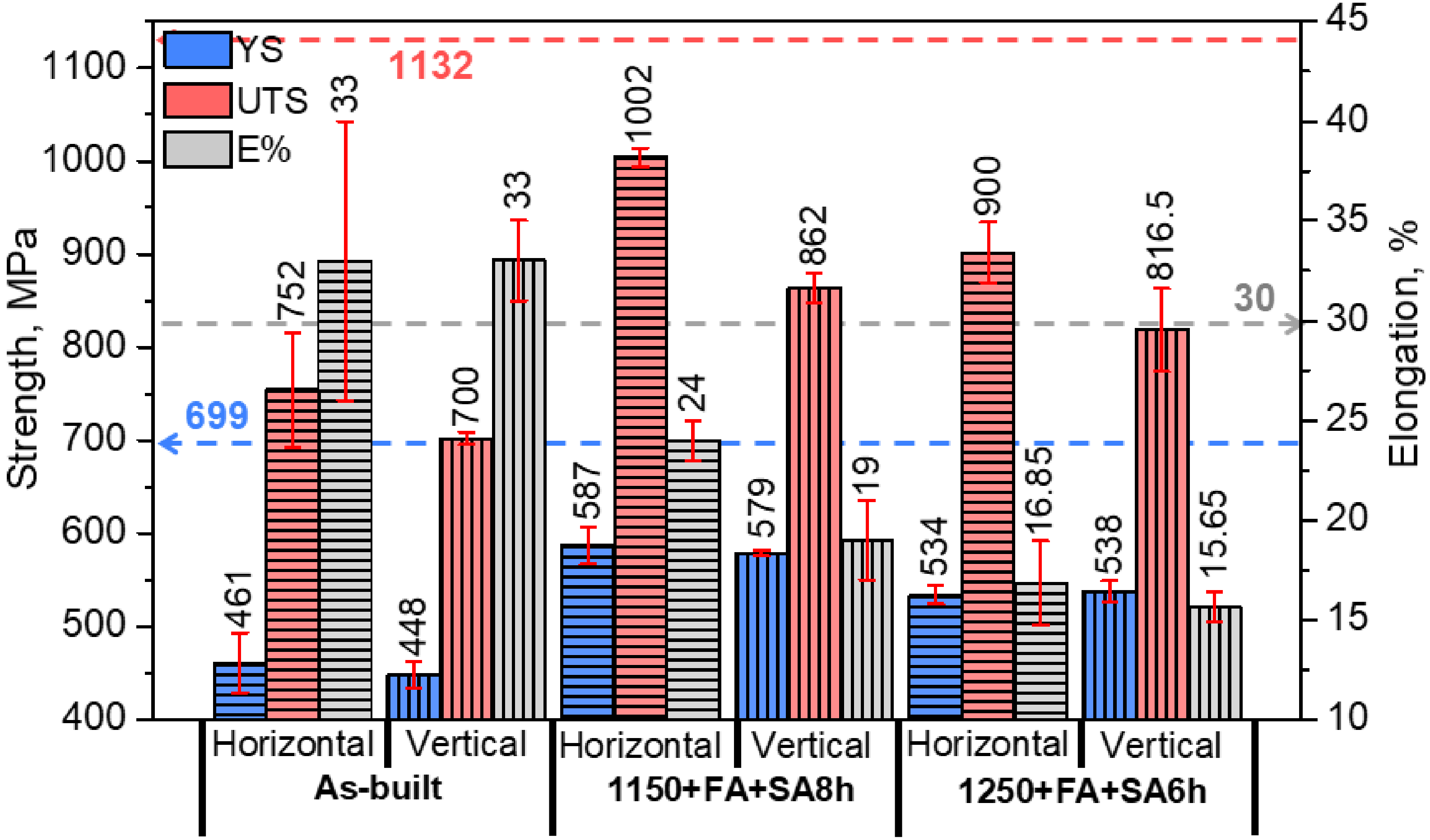
(a) **ST1250-FA-SA *x*h**



(b) **ST1150-FA-SA *x*h**



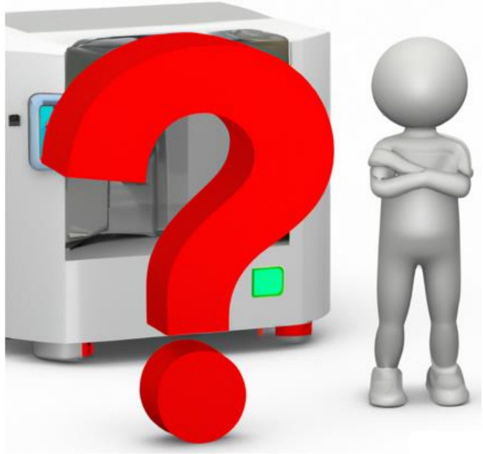
Tensile test results



FA: First aging, SA: Second aging

- The tensile test was performed on the samples with the highest hardness.
- Samples 1150-FA-SA8h and 1250-FA-SA6h did not reach the UTS, YS and Elongation of the Haynes 282 processed by forging.
- The low strength of Haynes 282 is attributed to porosity from the WAAM process.

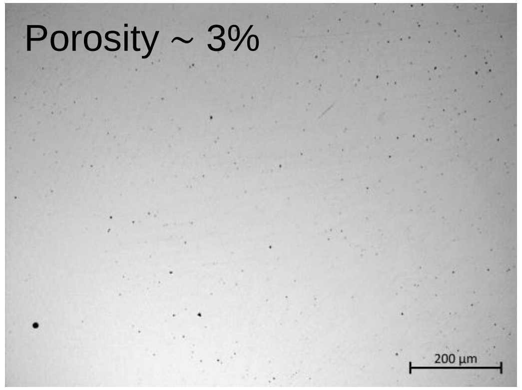
Why we have even worse yield strength with high hardness?



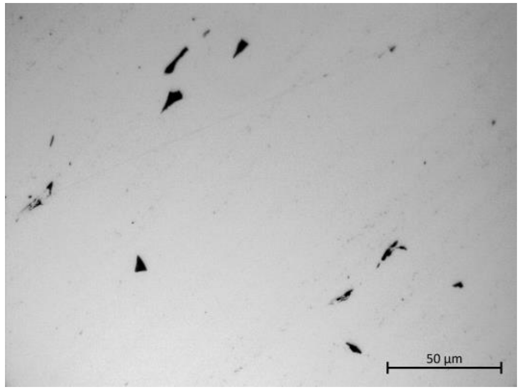
Porosity: as-built condition

As-built

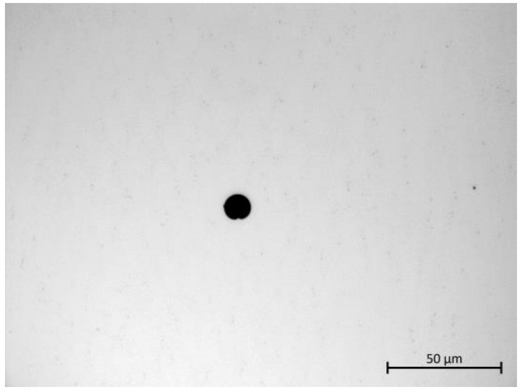
General view



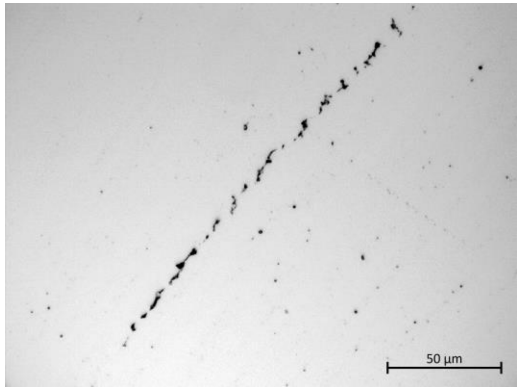
Lack-of-fusion pore



Gas pore



Solidification cracks



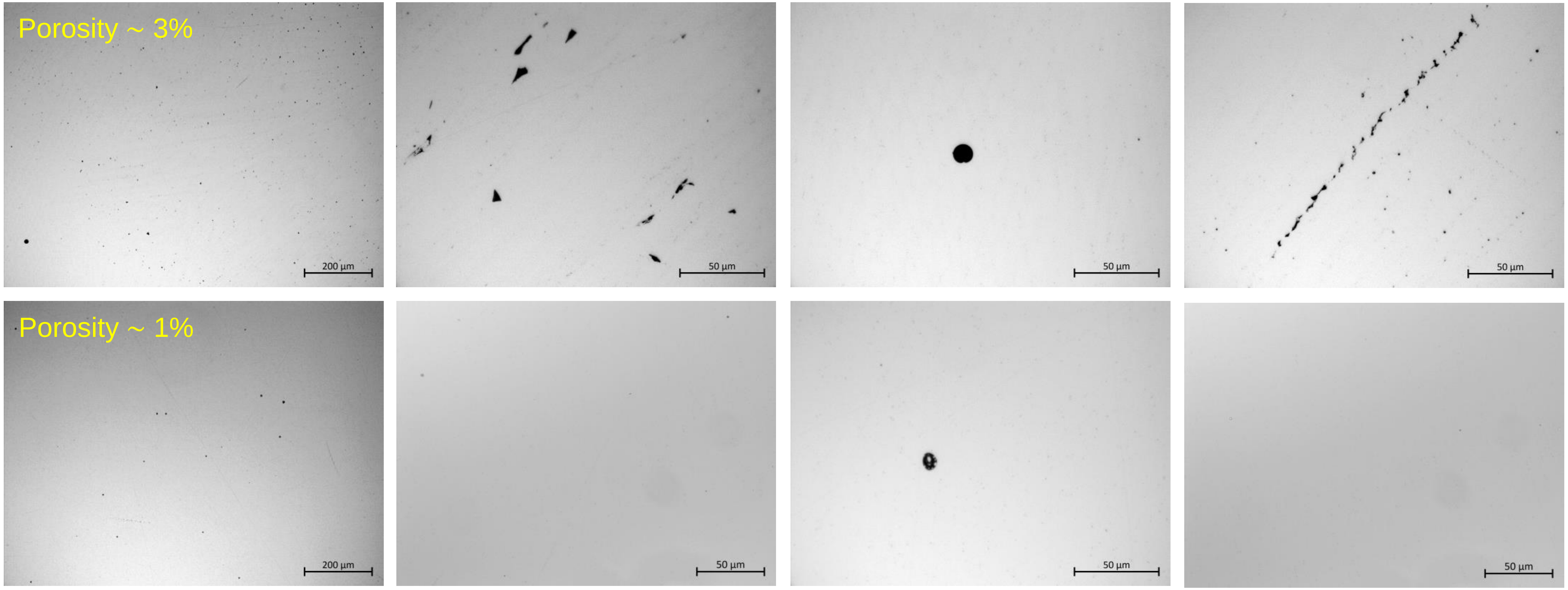
- As-built samples show porosity due to lack of fusion and gas. In addition, cracks of solidification were located.

Porosity: before and after HIP

General view | Lack-of-fusion pore | Gas pore | Solidification cracks

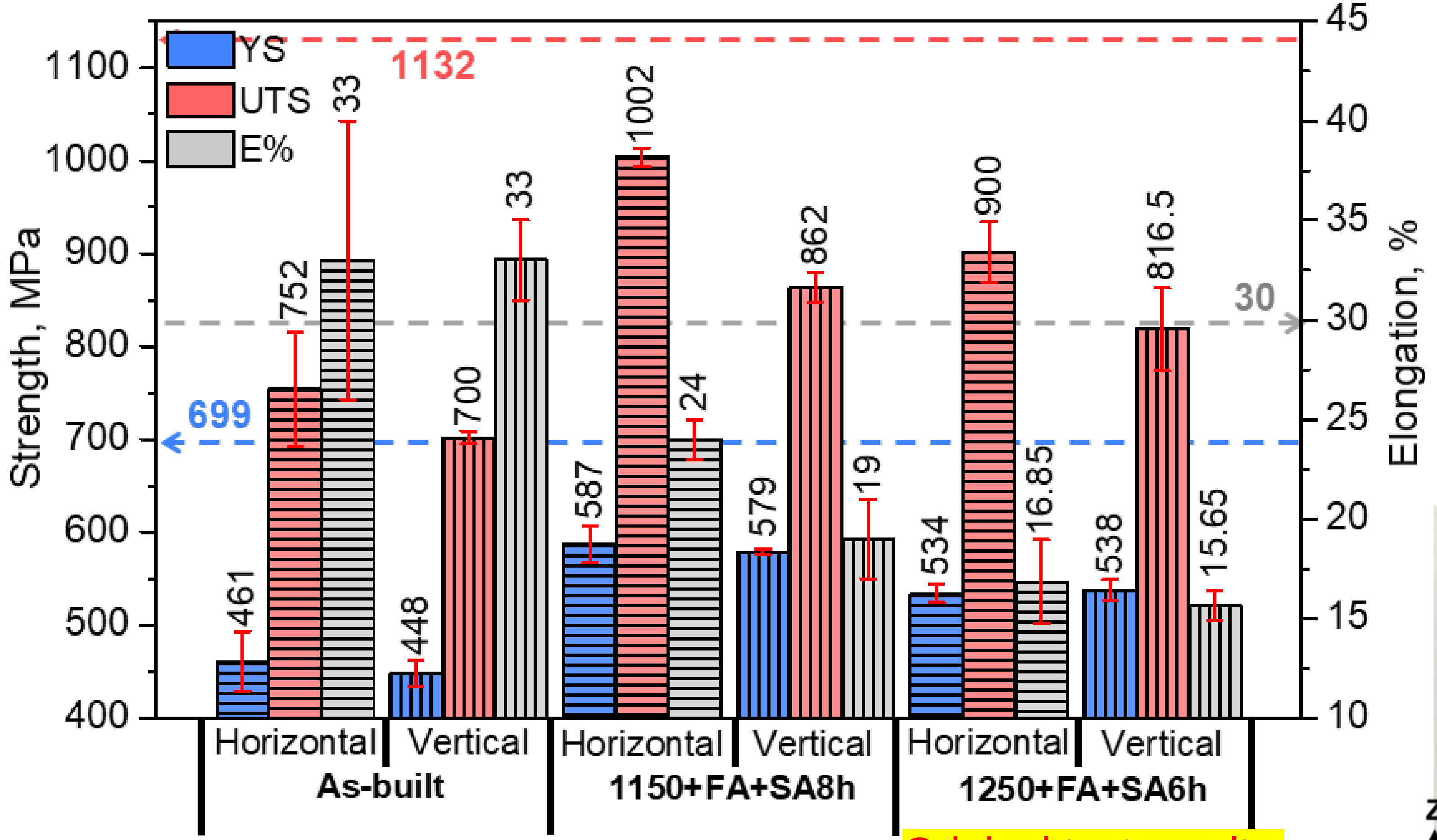
As-built

HIP

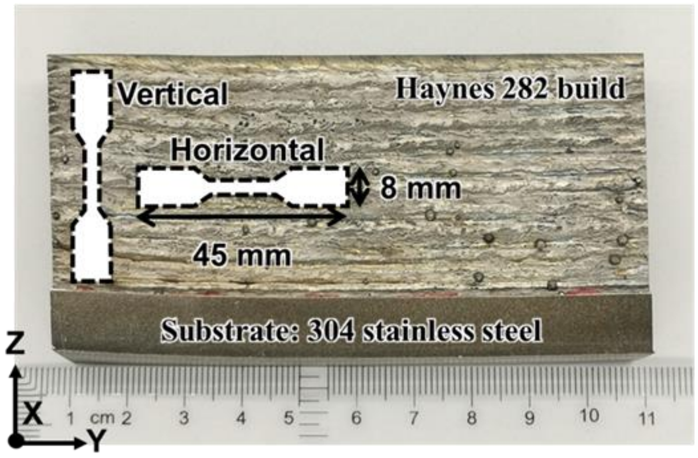


- As-built samples show porosity due to lack of fusion and gas. In addition, cracks of solidification were located.
- Samples after HIP show only gas pores.

Tensile test on samples w/o HIP

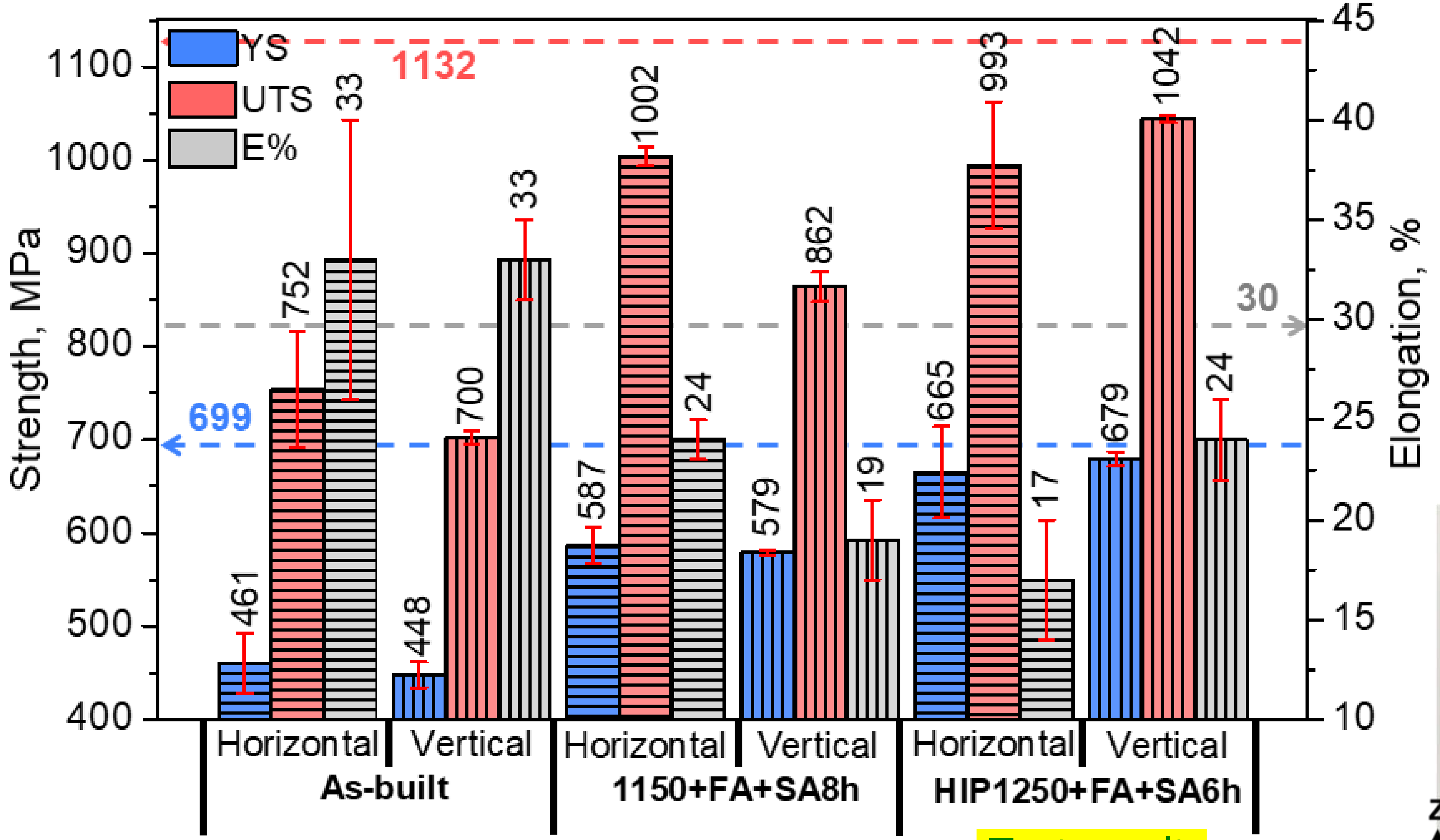


Original test results w/o HIP

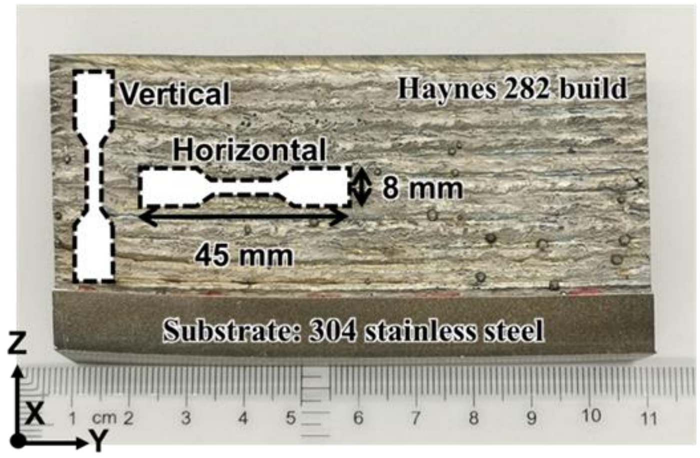


FA: First aging, SA: Second aging

Tensile test on samples with HIP

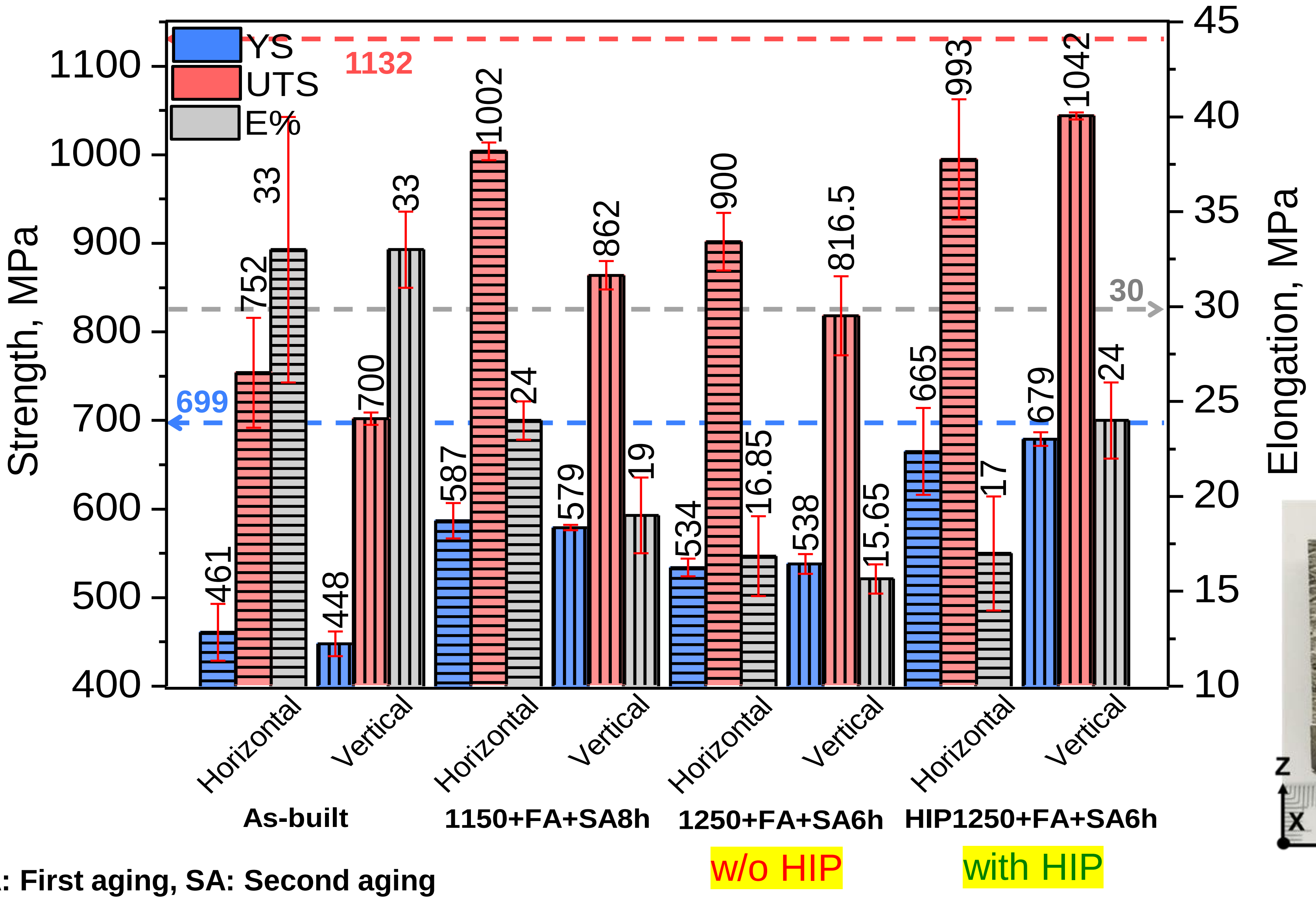


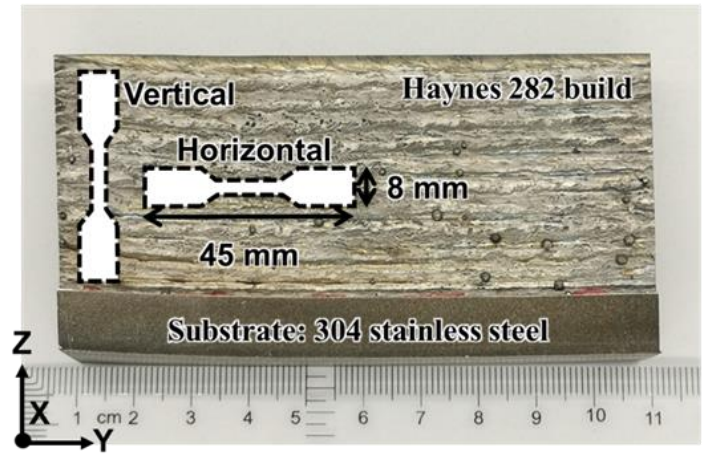
Test results with HIP



FA: First aging, SA: Second aging

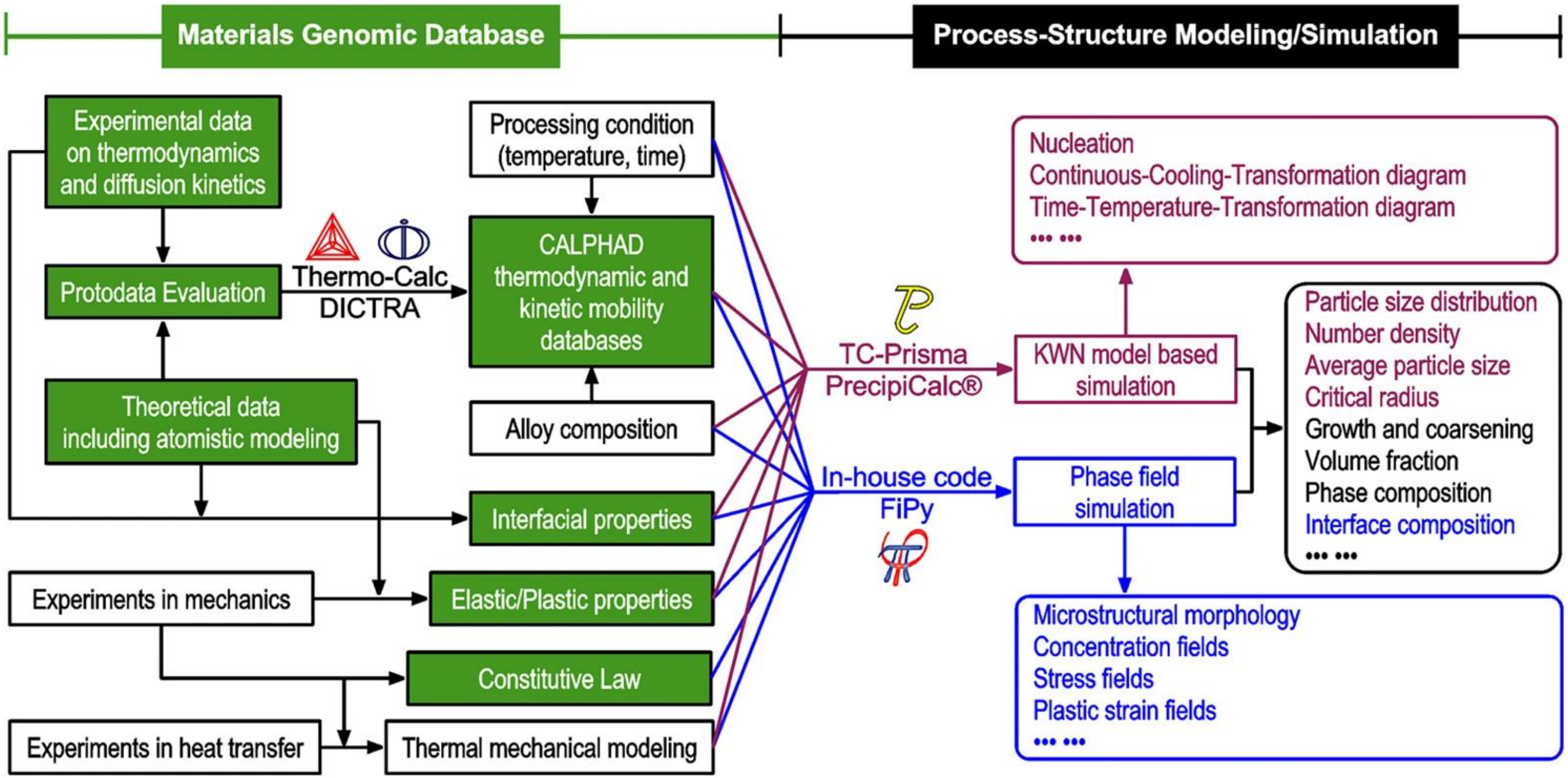
Tensile test with vs. without HIP





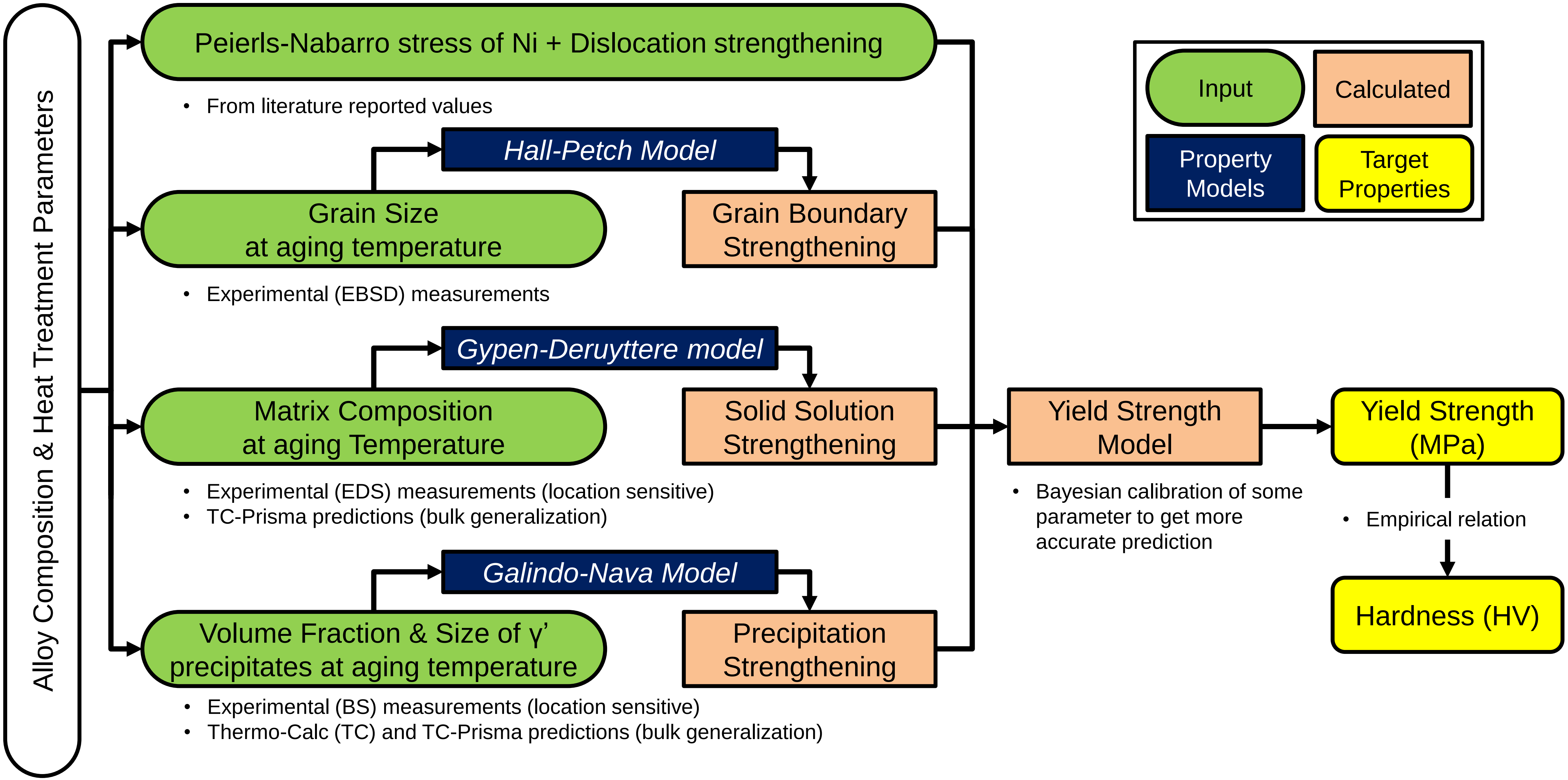
FA: First aging, SA: Second aging

CALPHAD-based ICME modeling of precipitation kinetics



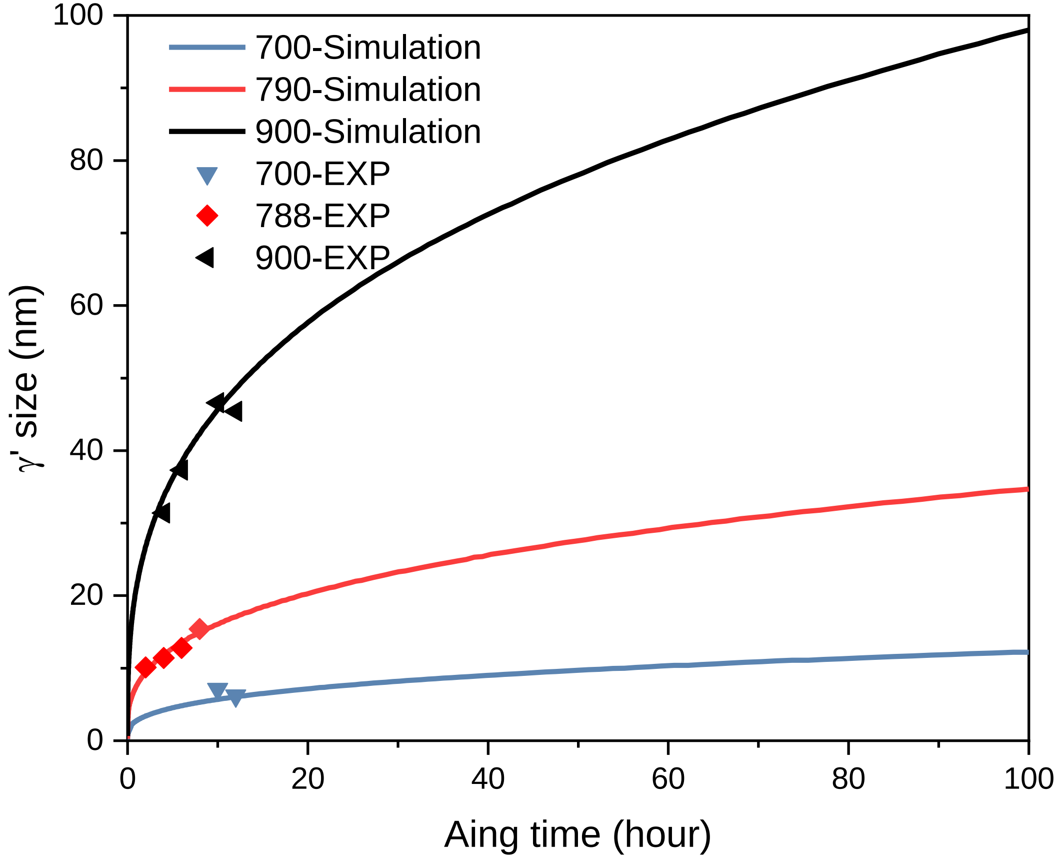
Wei Xiong, Gregory B. Olson, *npj Computational Materials*, nature publishing group, 2 (2016) 15009.

ICME Yield Strength Model Overview



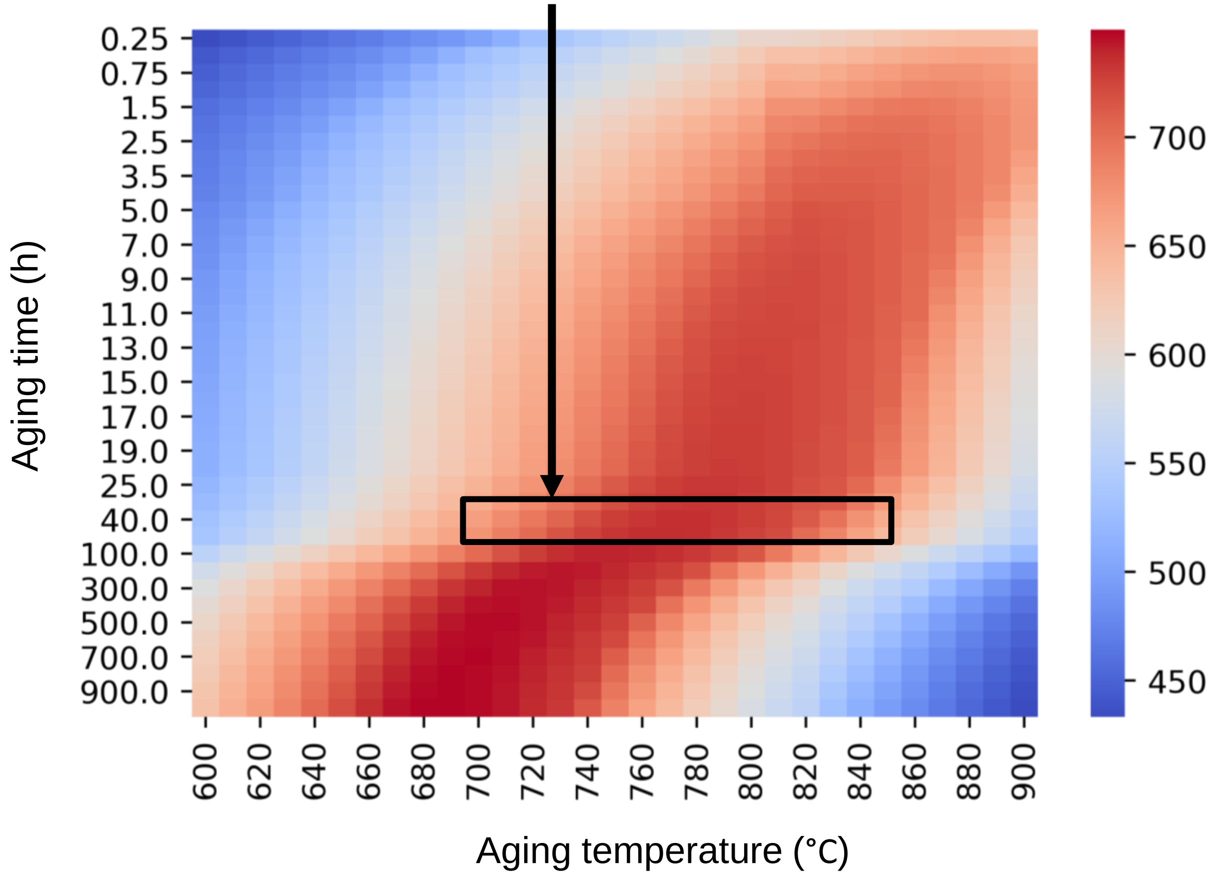
Interfacial Energy Calibration and Yield Strength Prediction

Simulated γ' size matches experiments

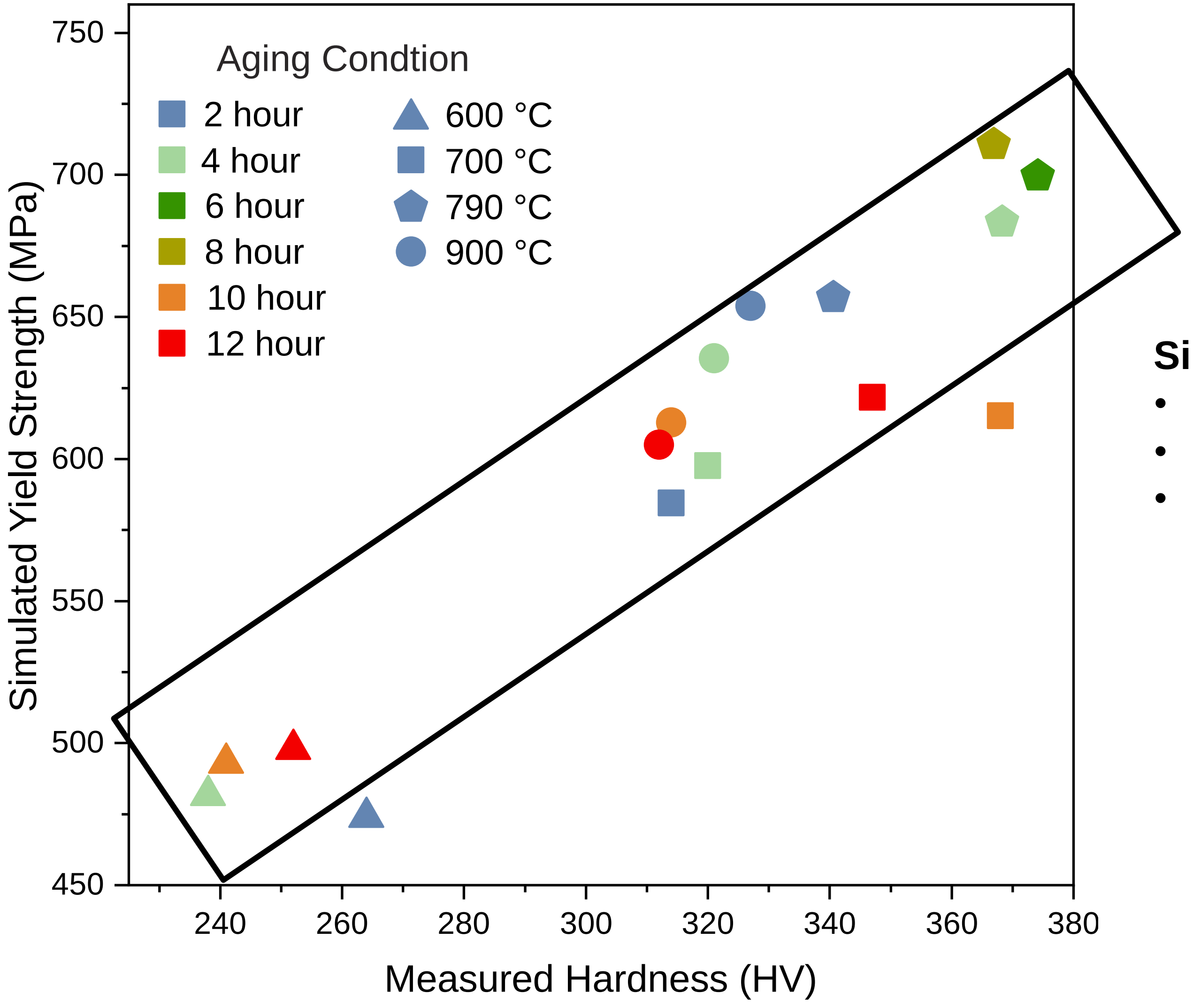


NB: Experiments performed are the ones w/o HIP

Desired yield strength can be achieved in less than 50 hours in the temperature range of 700-850°C, although long-time aging can help to further improve the strength.



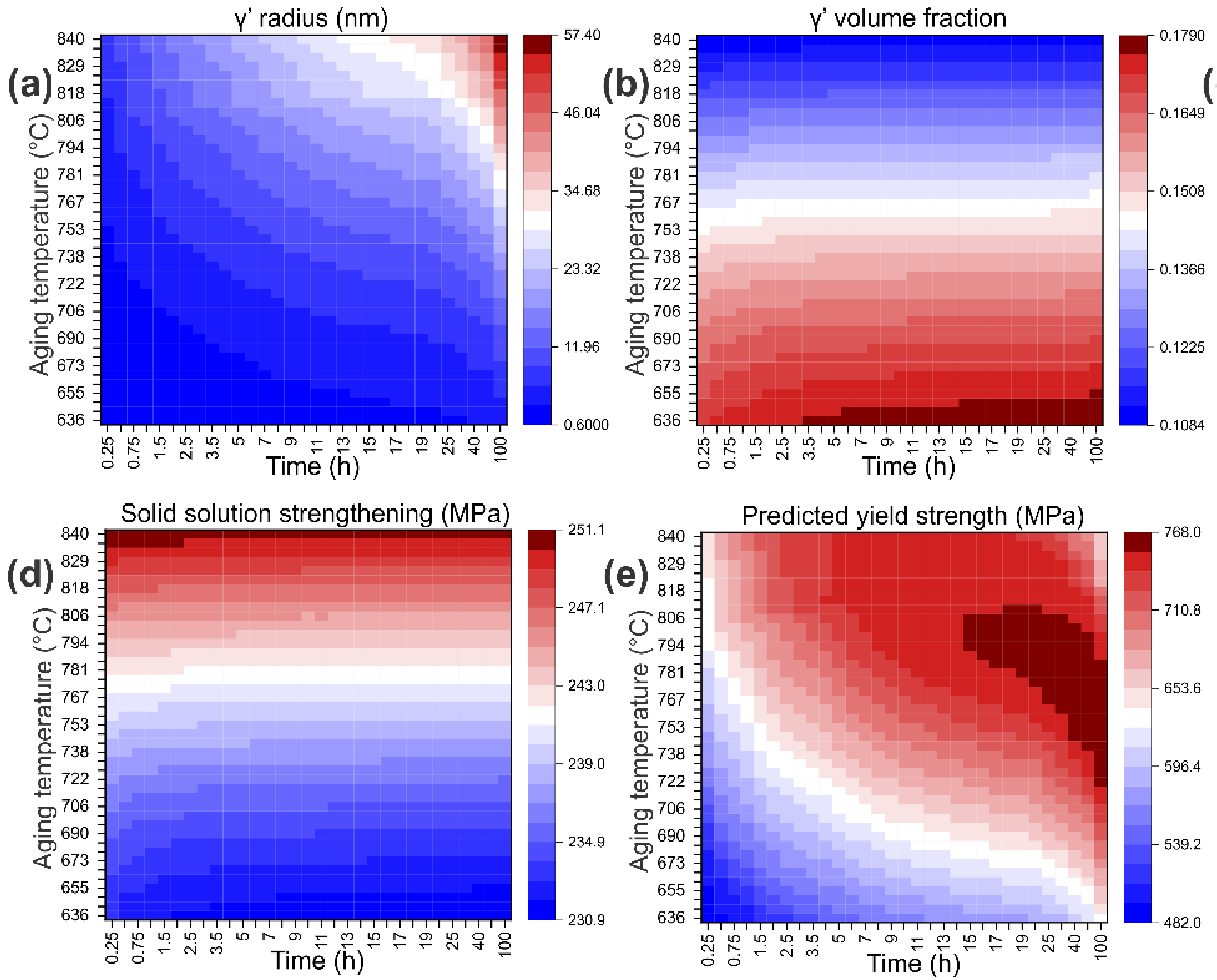
Predicted Yield Strength vs. Hardness Data



Simulation vs. Experiments:

- Model prediction matches experiments
- Simulated yield strength ≈ **2** x Measured hardness
- 790 °C aging is the optimized condition

CALPHAD-based ICME model prediction after calibration using experiments



Now we can use the CALPHAD-based ICME results to guide high-throughput experimentation

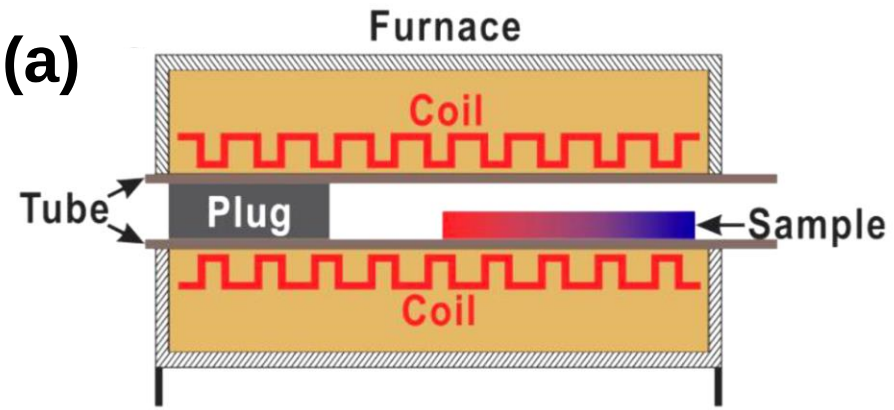
High-throughput experiments supporting ICME-ML design of yield strength

To generate data for machine learning and find the peak hardness of Haynes 282 samples, a graded heat treatment was performed.

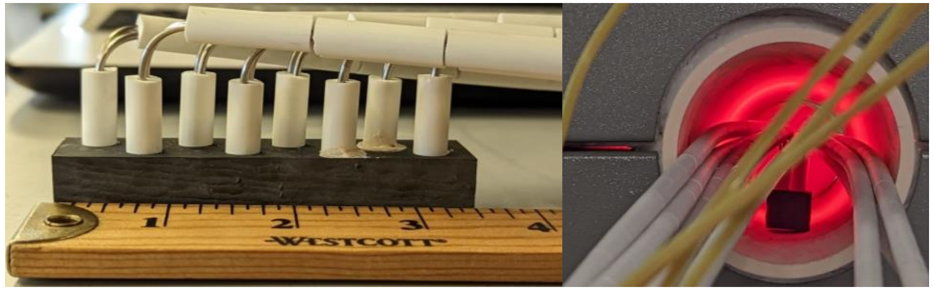
We applied HIP on high-throughput samples

- The studied temperature range is 650°C-850°C
- The aging times are 6 and 50 hours.

(a)

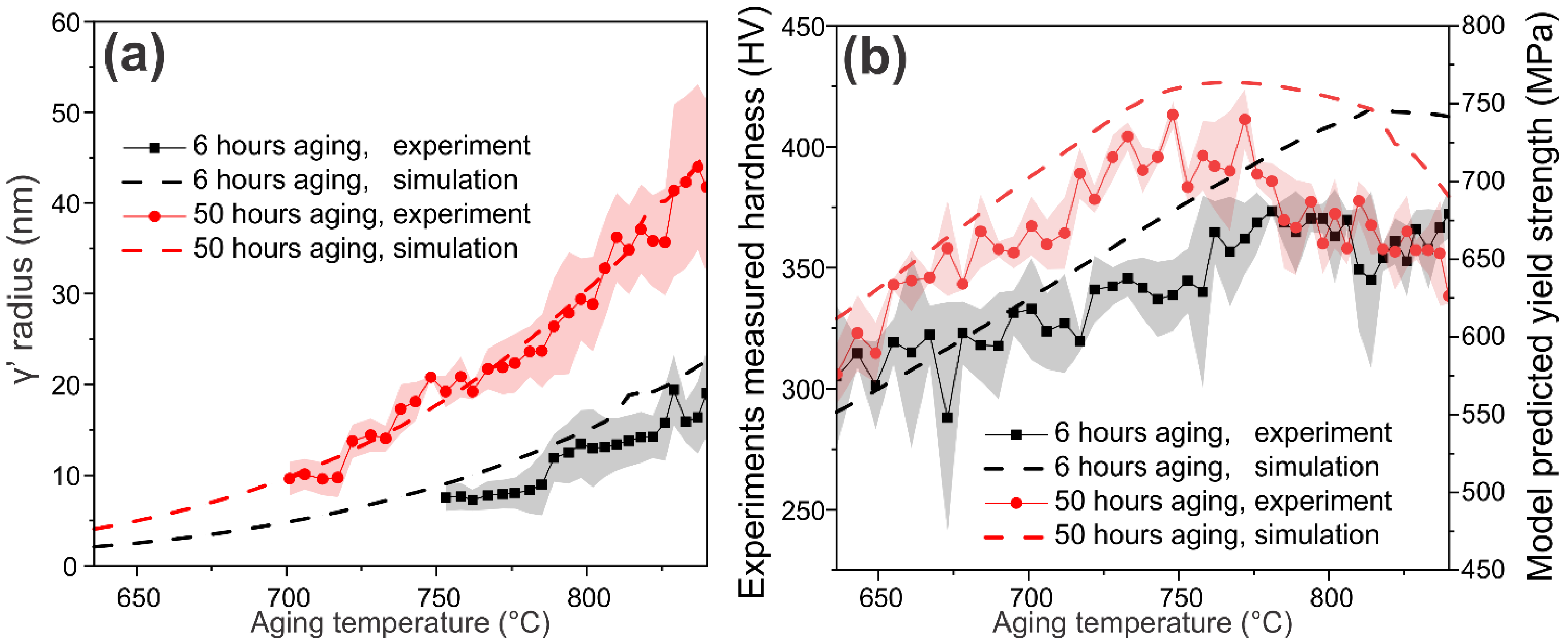


(b)



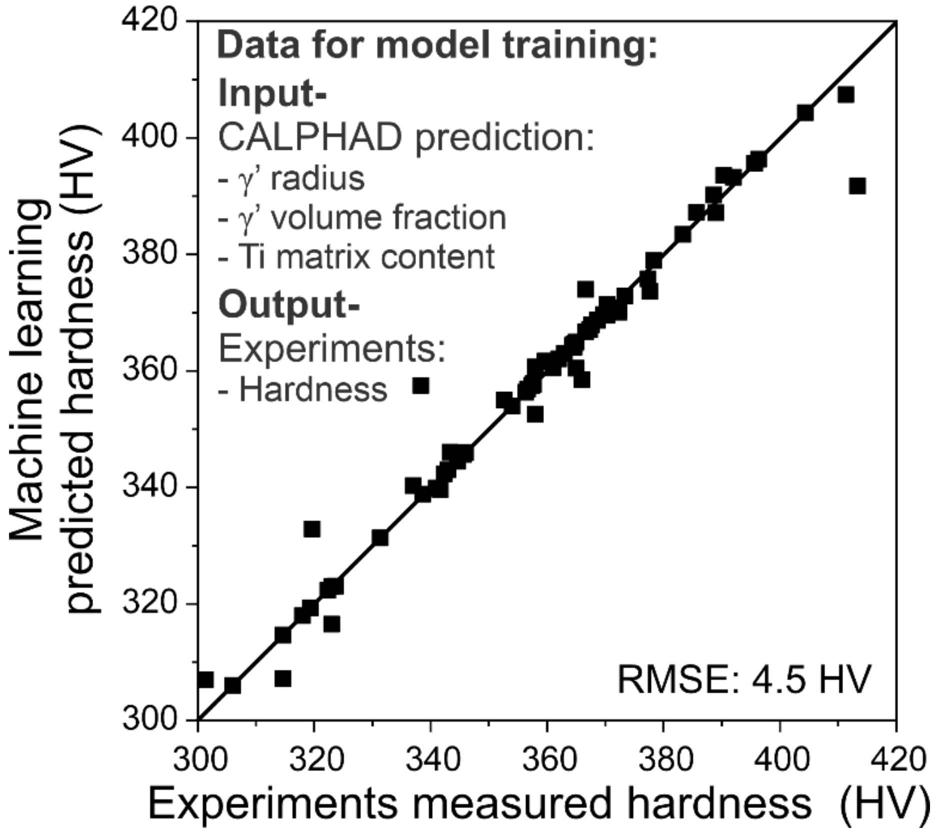
Ref.: Yunhao Zhao, ..., Wei Xiong, "***A new high-throughput method using additive manufacturing for alloy design and heat treatment optimization***", ***Materialia***, 13 (2020) 100835.

CALPHAD-based simulation of precipitation kinetics



Machine learning prediction of hardness

- In the modeling process, the hardness data with a standard deviation larger than 20 HV were removed as outliers.
- We performed the correlation study of the matrix composition to remove the highly correlated features as this will reduce the model complexity and avoid overfitting.

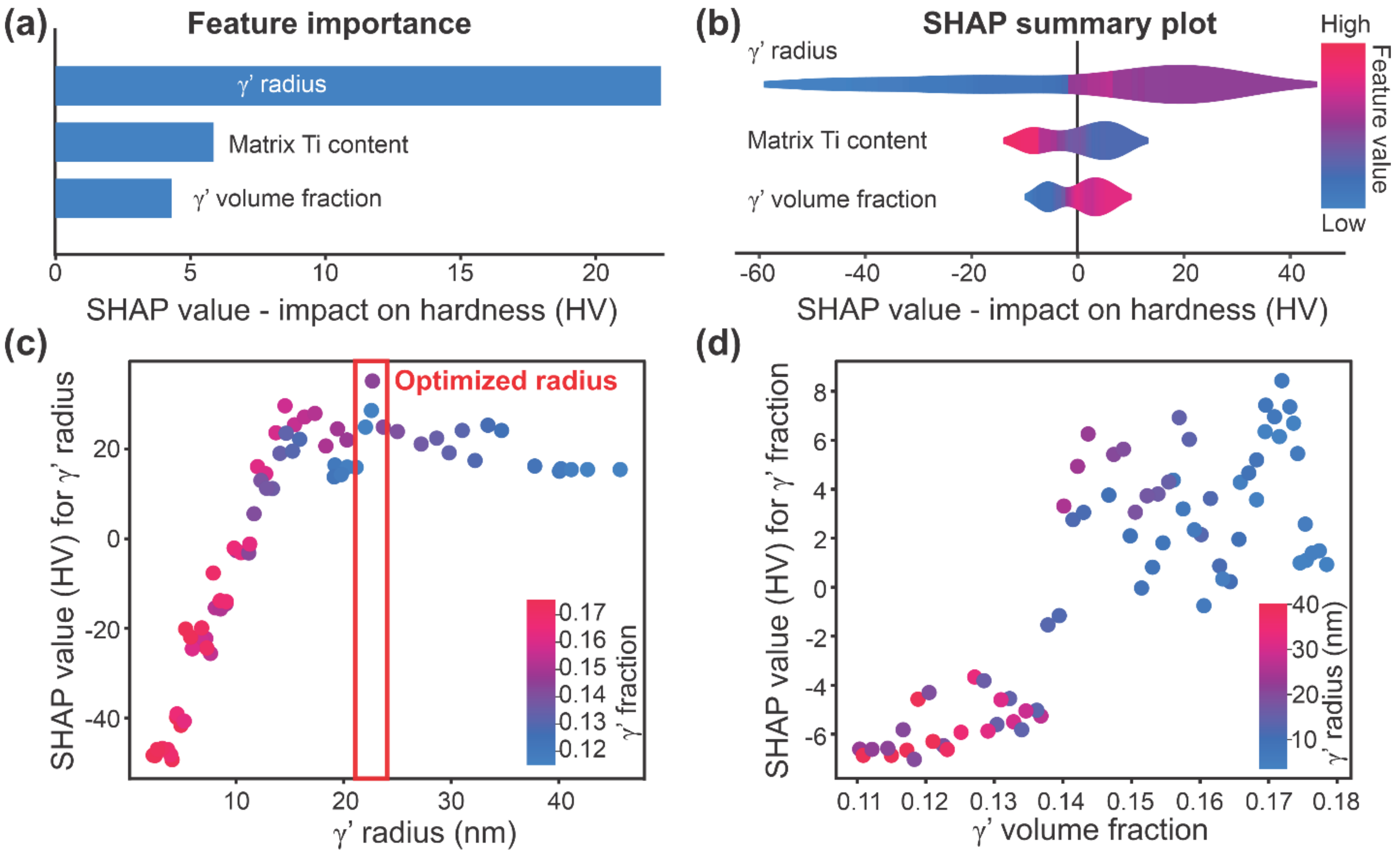


Pearson correlation coefficients between the matrix composition calculated using CALPHAD approach

	Al	Co	Cr	Fe	Mn	Mo	Si	Ti	Ni
Al	1	-0.999	-0.999	-0.997	-0.999	-0.999	-0.998	0.996	0.999
Co	-0.999	1	1	0.999	1	1	1	-0.999	-1
Cr	-0.999	1	1	0.999	1	1	1	-0.999	-1
Fe	-0.997	0.999	0.999	1	0.999	1	1	-1	-0.999
Mn	-0.999	1	1	0.999	1	1	1	-0.998	-1
Mo	-0.999	1	1	1	1	1	1	-0.999	-1
Si	-0.998	1	1	1	1	1	1	-0.999	-1
Ti	0.996	-0.999	-0.999	-1	-0.998	-0.999	-0.999	1	0.999
Ni	0.999	-1	-1	-0.999	-1	-1	-1	0.999	1

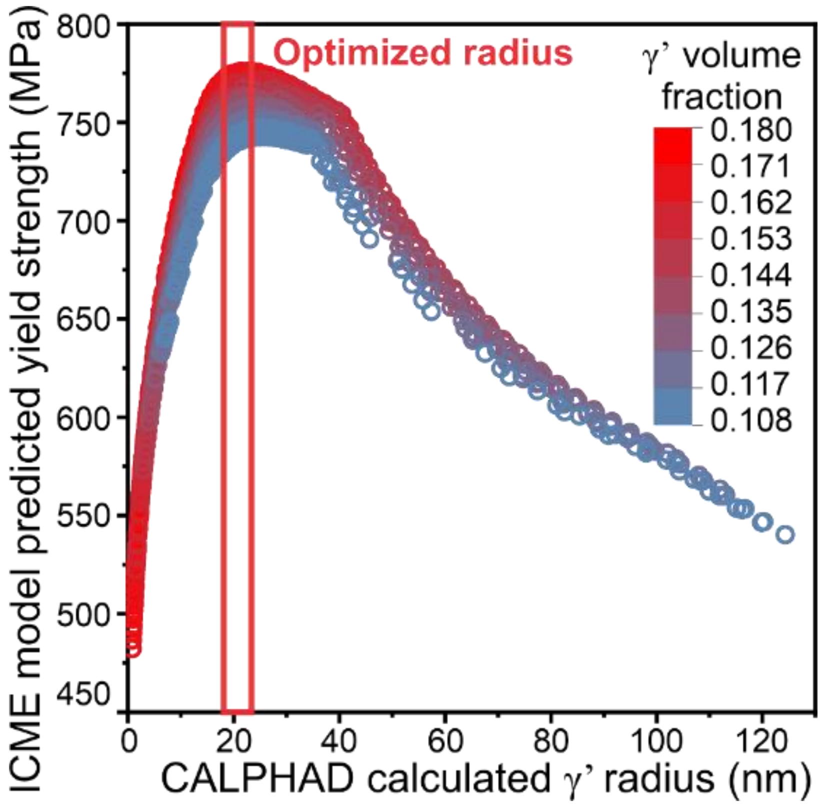
Interpret the machine learning model using SHAP and heat treatment design

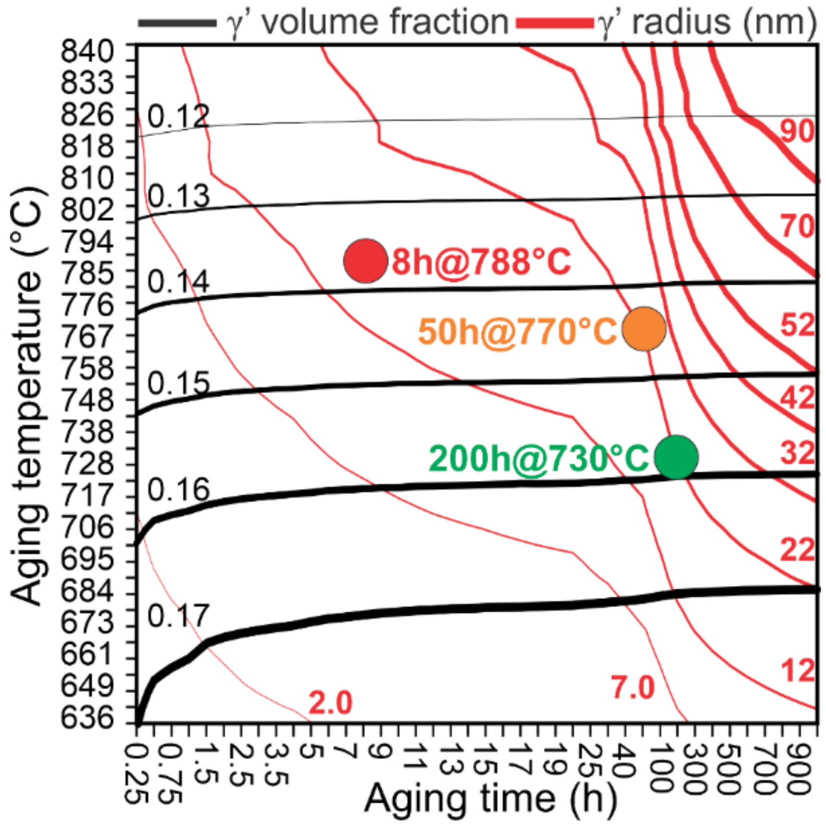
Phase fraction of γ' is less important than radius, as long as it reaches the desired range 14~18 vol.%.



CALPHAD-based ICME has the similar conclusion

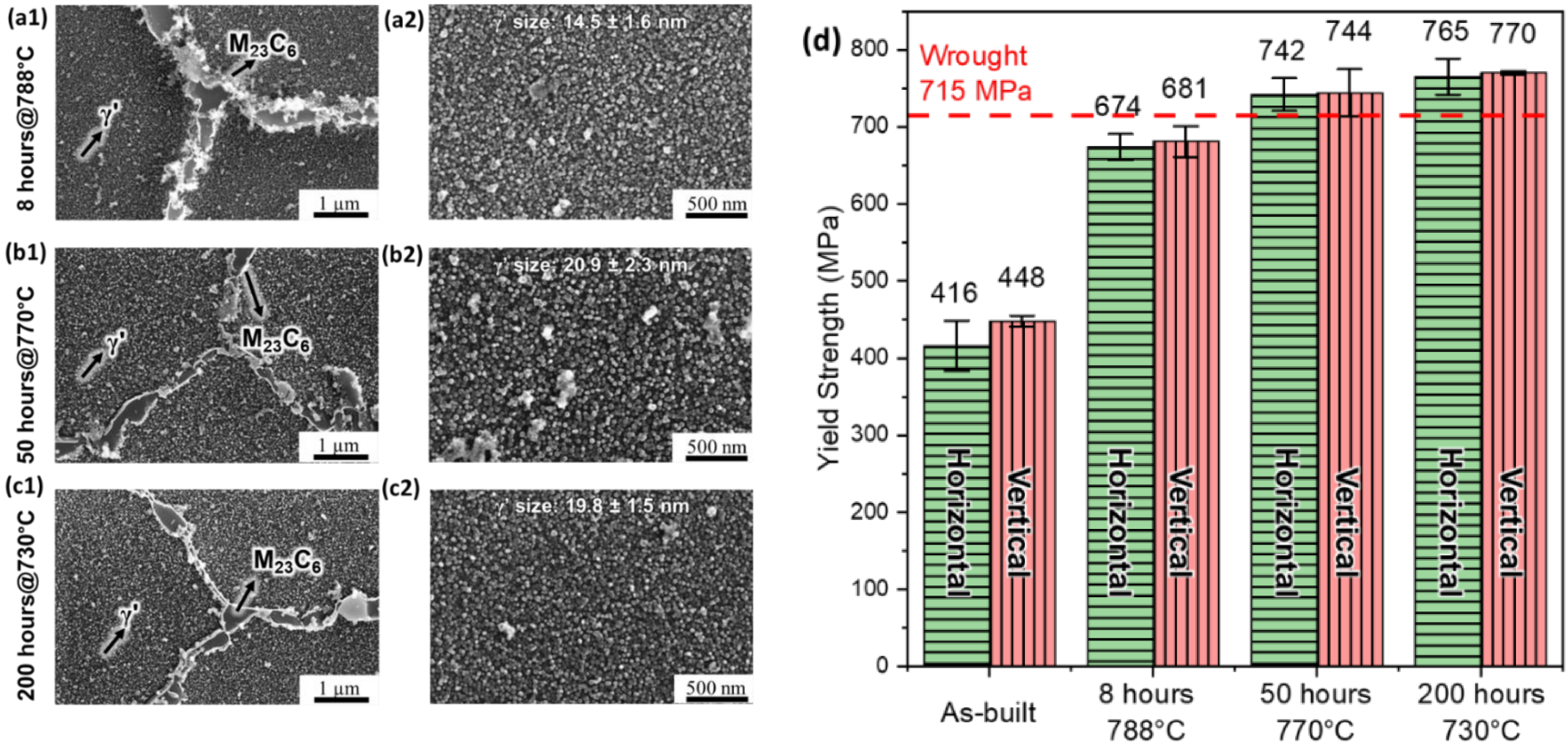
Phase fraction of γ' is less important than radius, as long as it reaches the desired range ~17%.



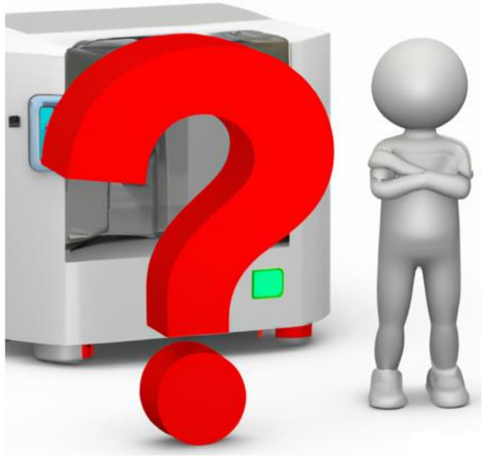


Contour plot of the CALPHAD calculated γ' size and volume fraction for aging time ranging from 0.25 to 1000 hours and temperature between 636 and 840 °C.

Microstructure and yield strength and after different 2nd aging heat treatments

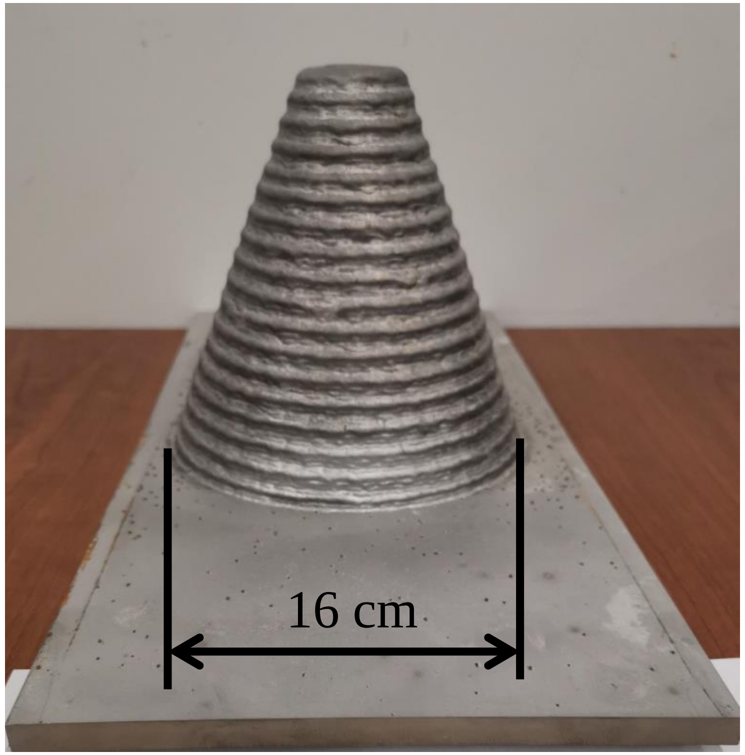


Can we also evaluate the location-specific properties with optimized heat treatment?

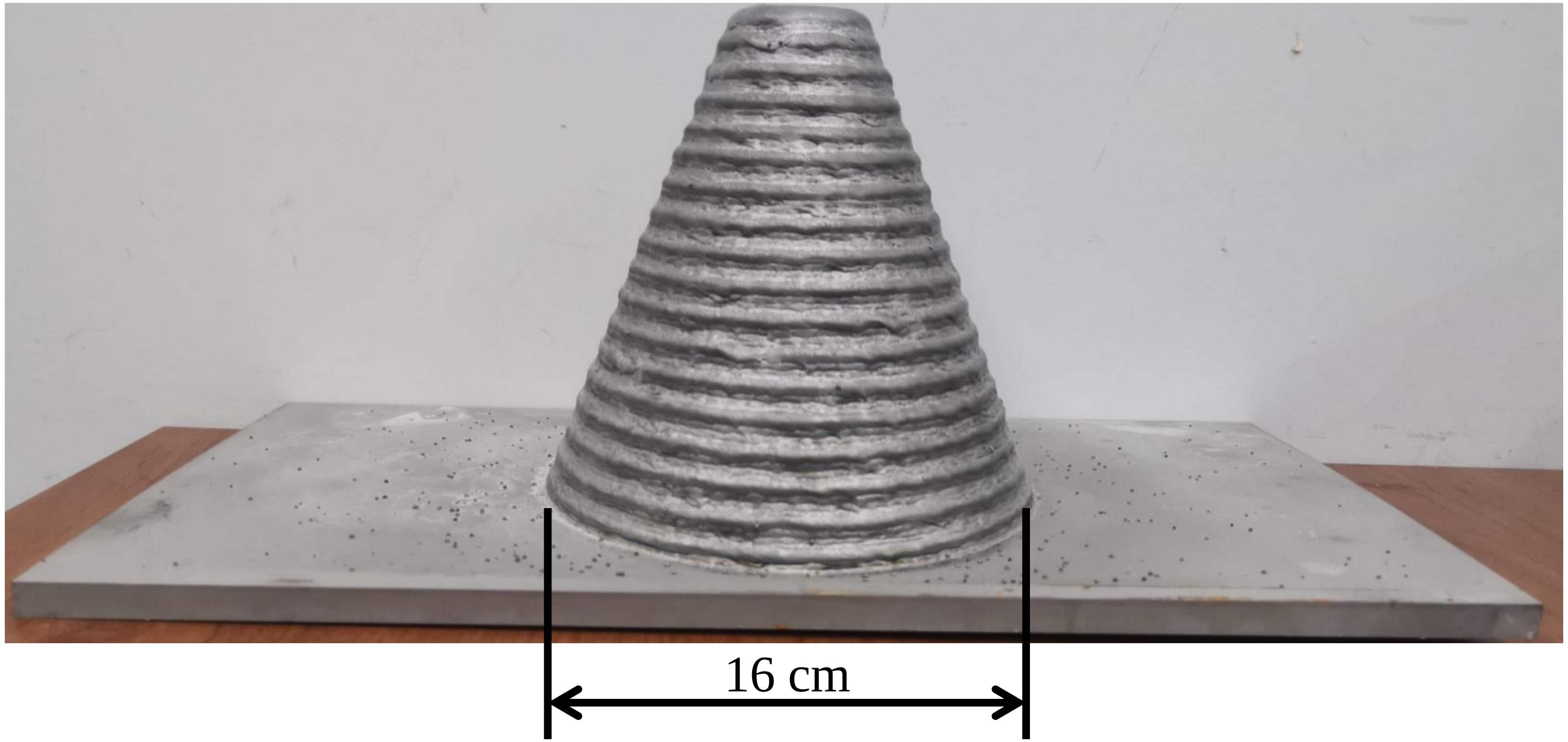


WAAM builds – Cone shape sample

Side view



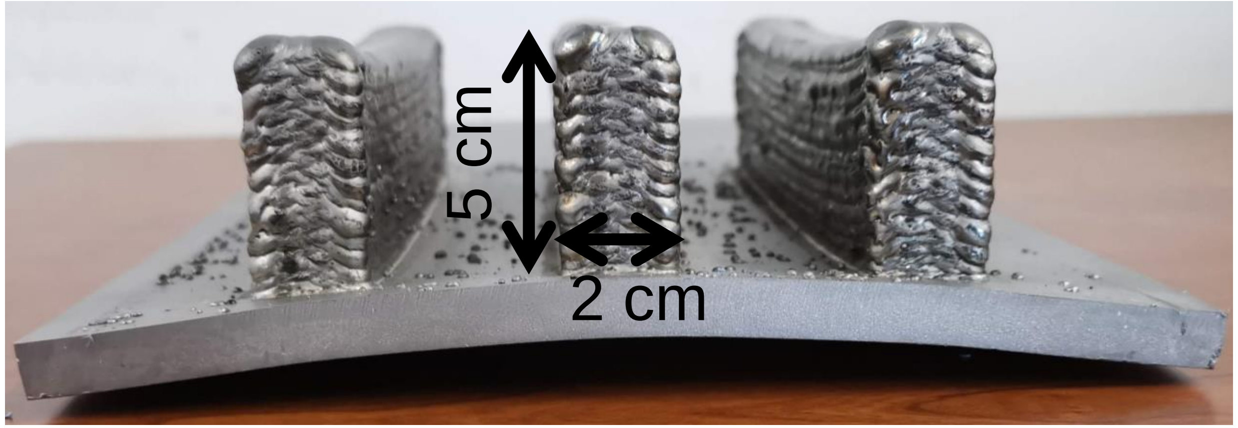
Front view



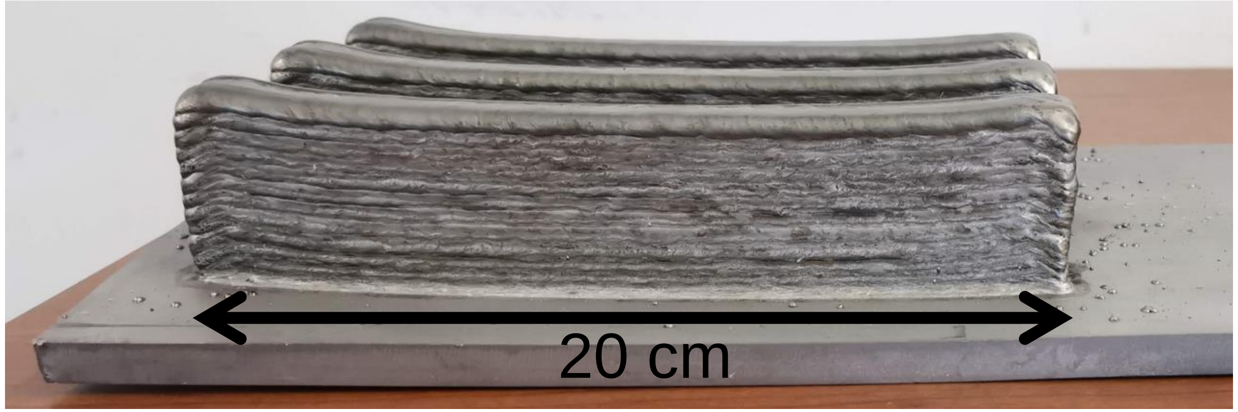
Cone build showed heavy distortion in the middle in comparison with the circumference

WAAM builds – Wall shape samples

Front view



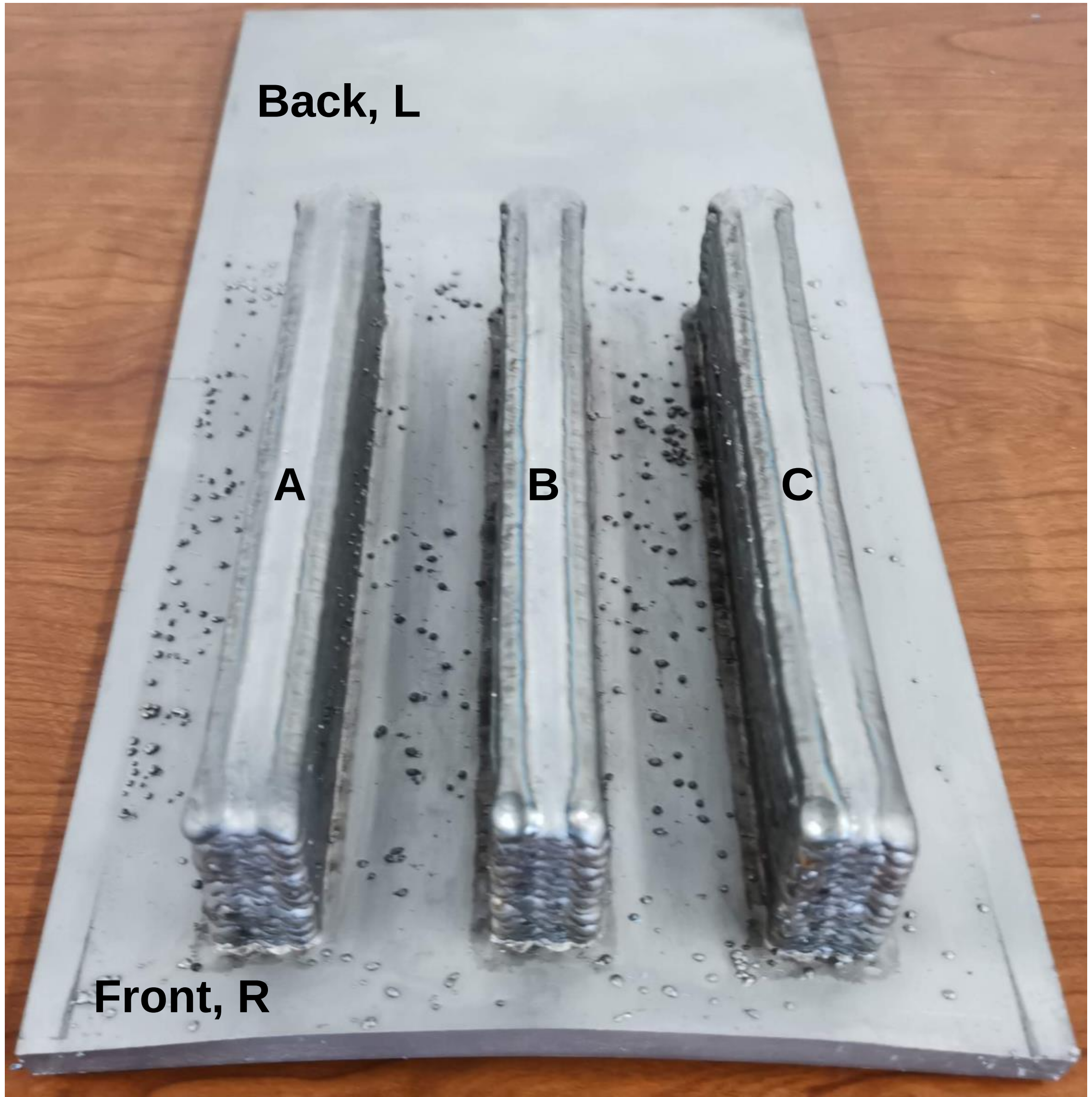
Side view



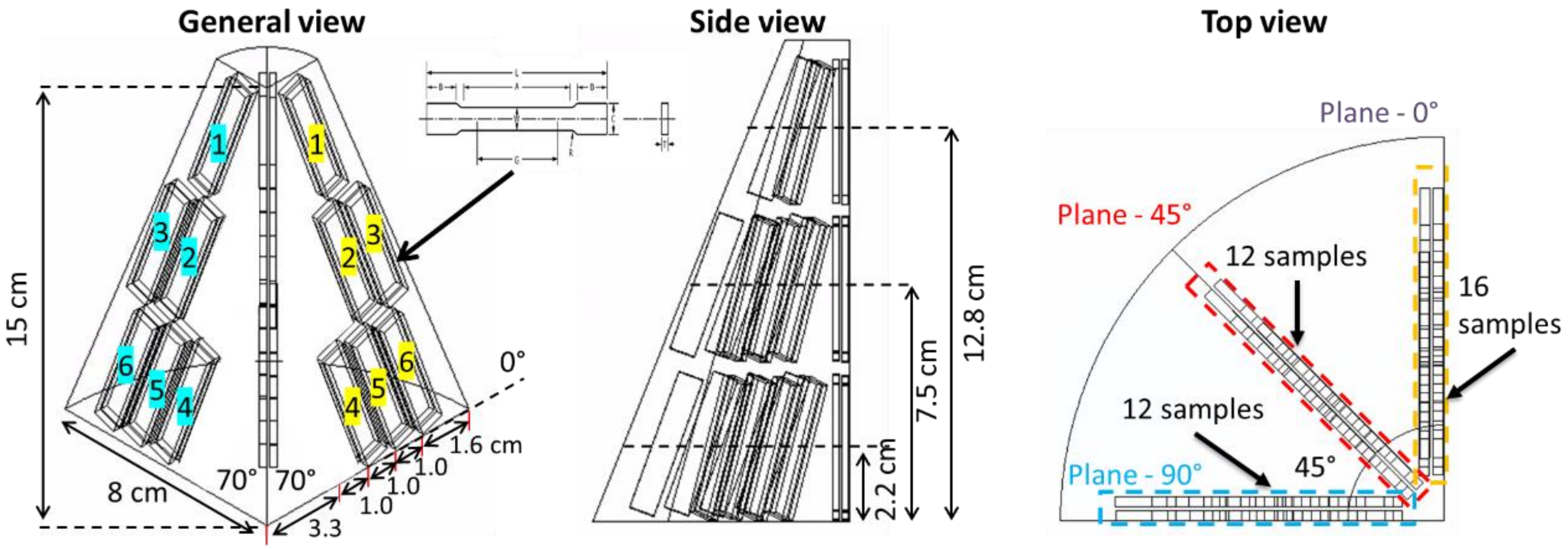
Single bead pattern

5 cm

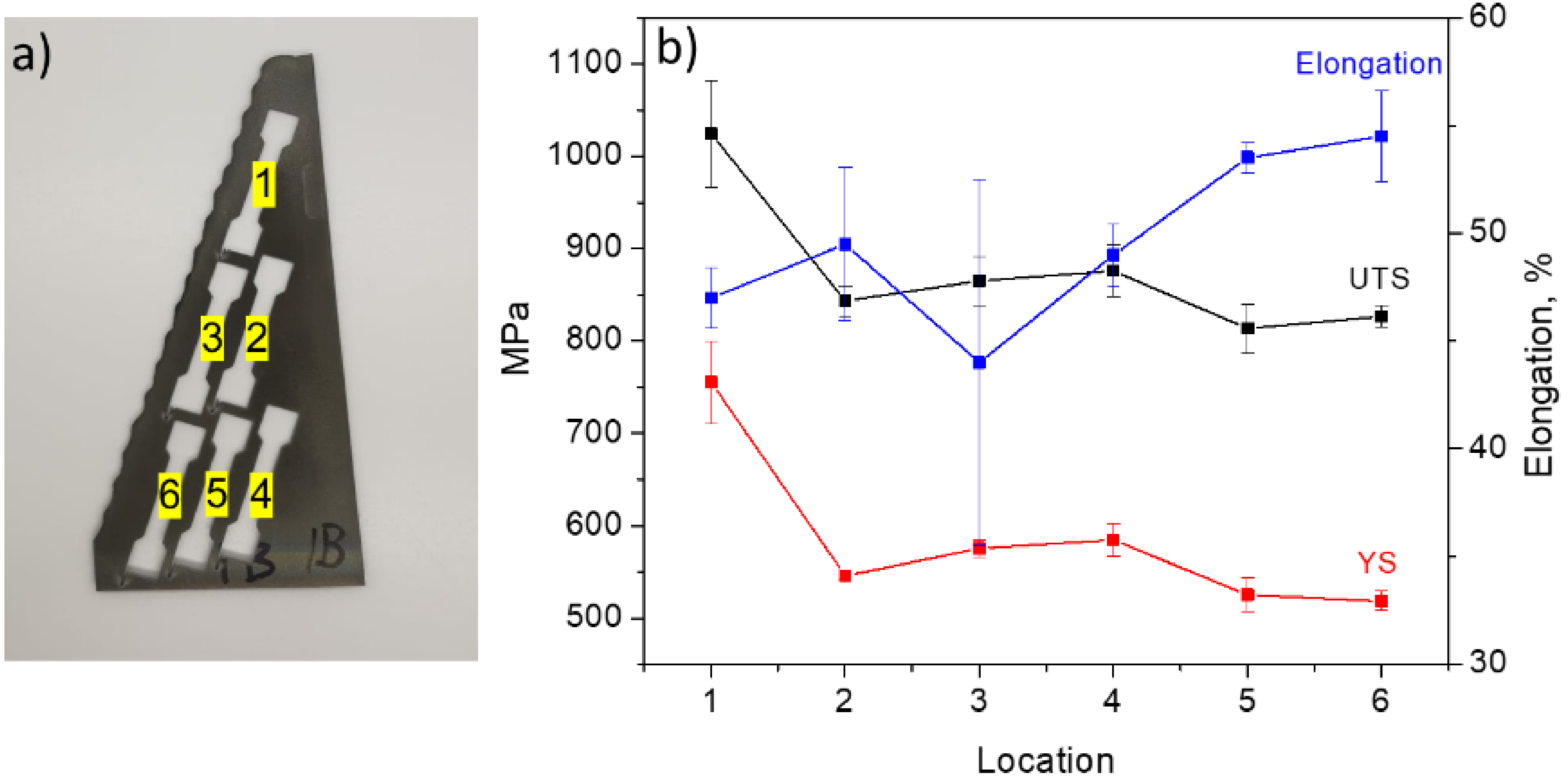
Top view



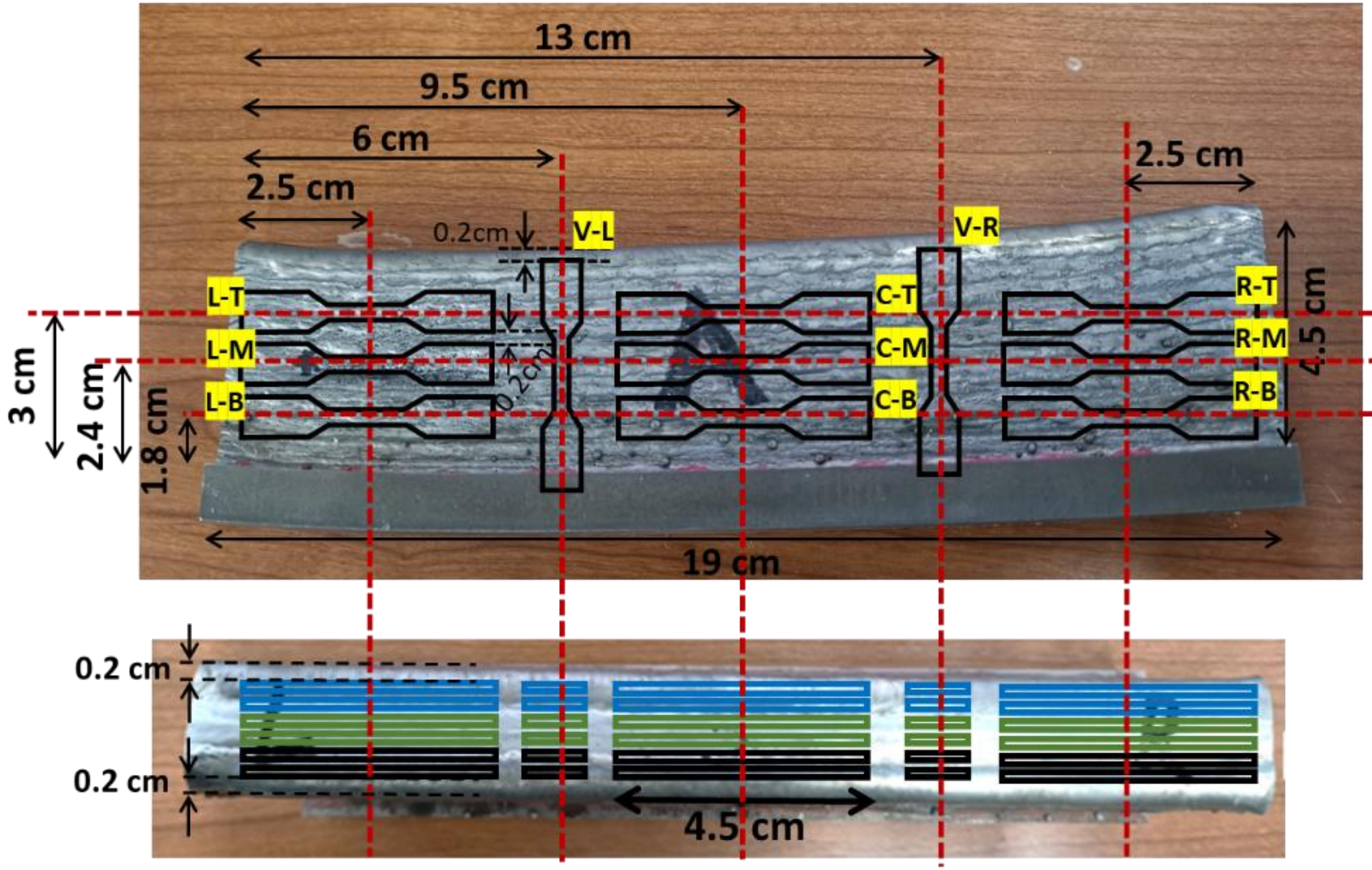
Cone shape sample: Cutting for location specific study

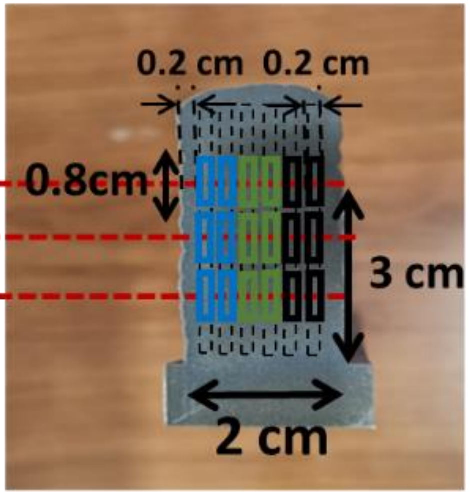


Cone shape sample: Cutting for location specific study (as-printed)

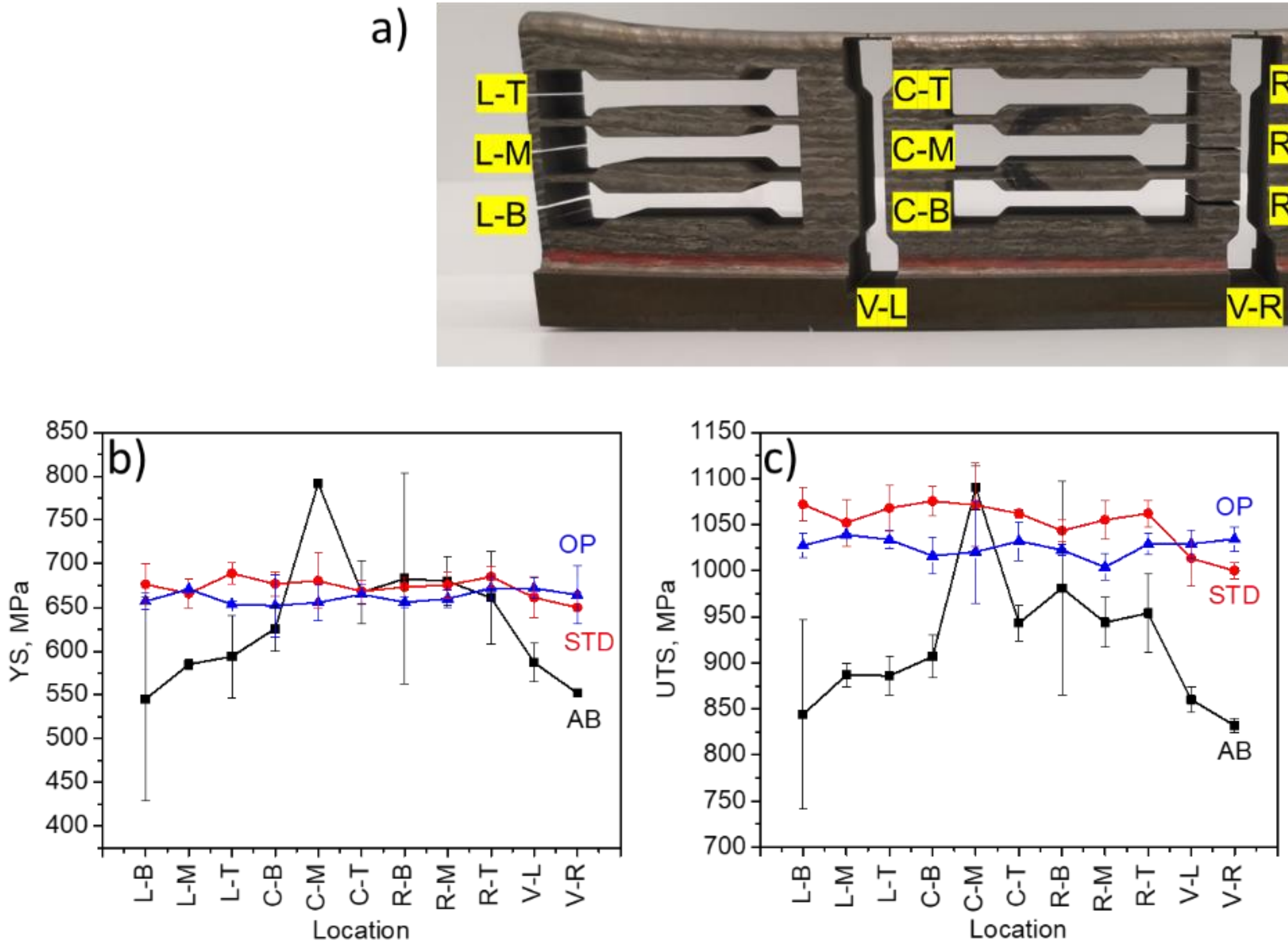


Wall shape sample: Cutting for location specific study





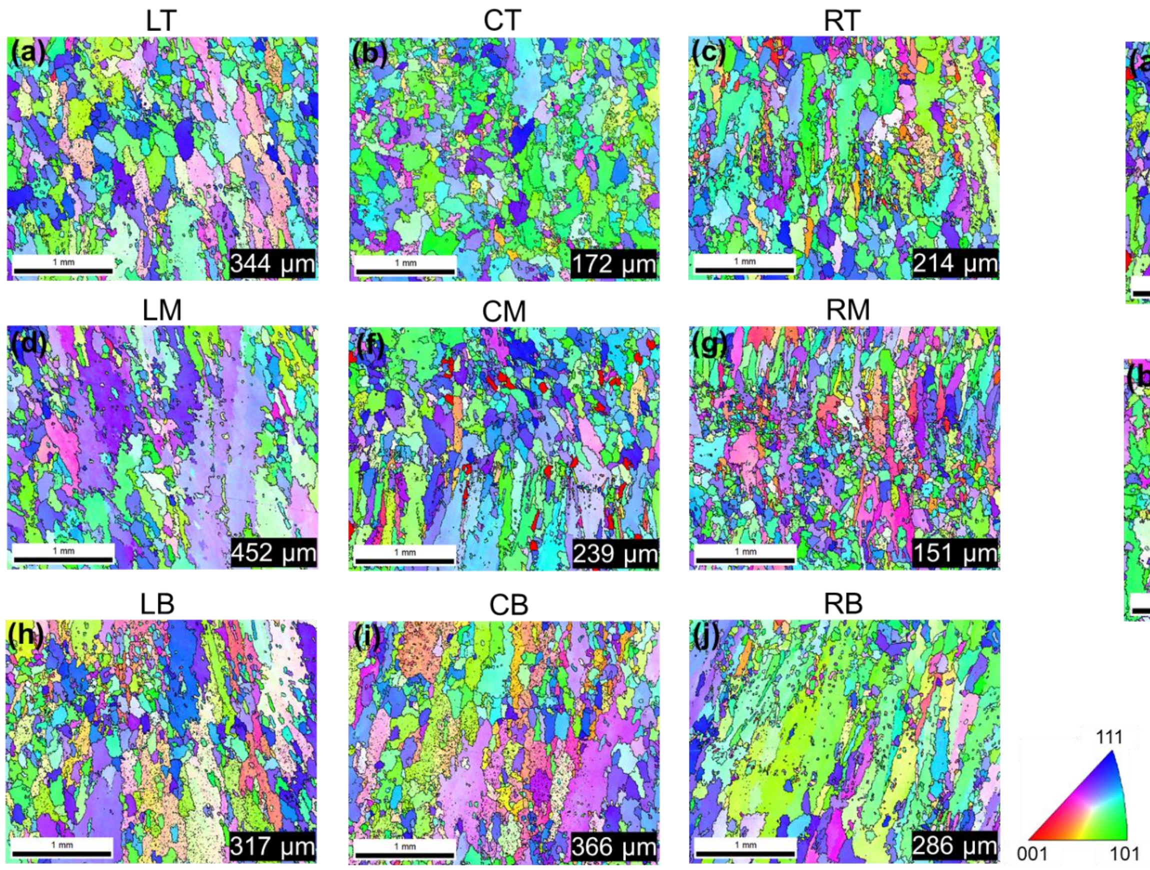
Wall shape sample: Cutting for location specific study



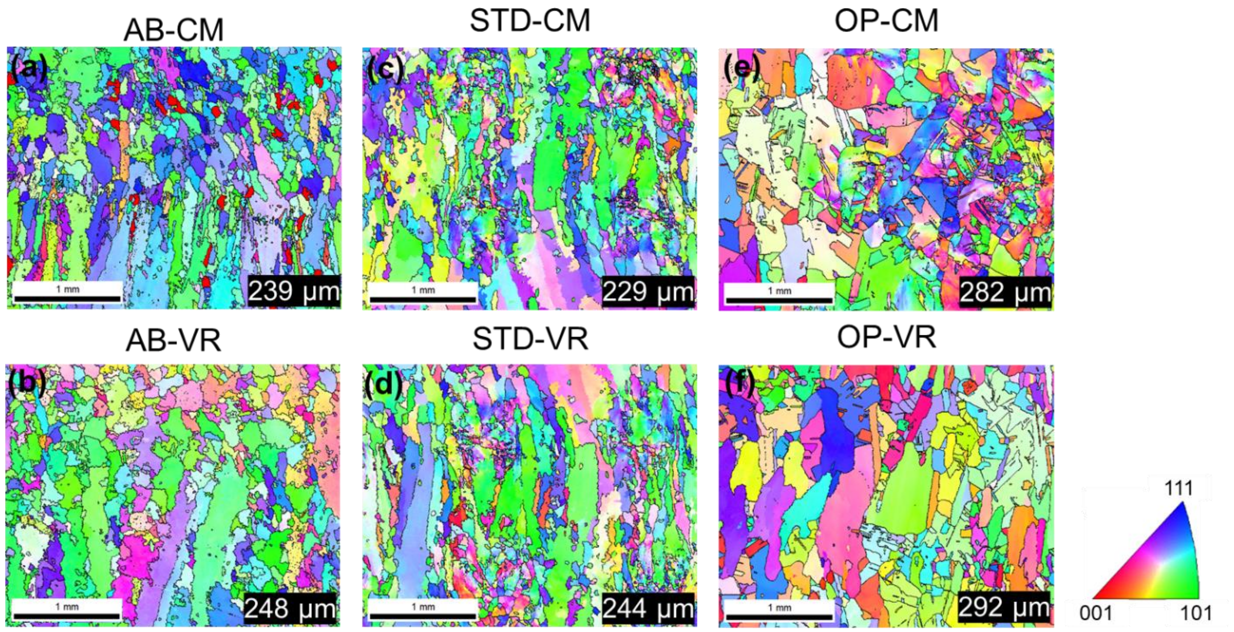
The optimized heat treatment can greatly reduce the heterogeneity of the printed sample

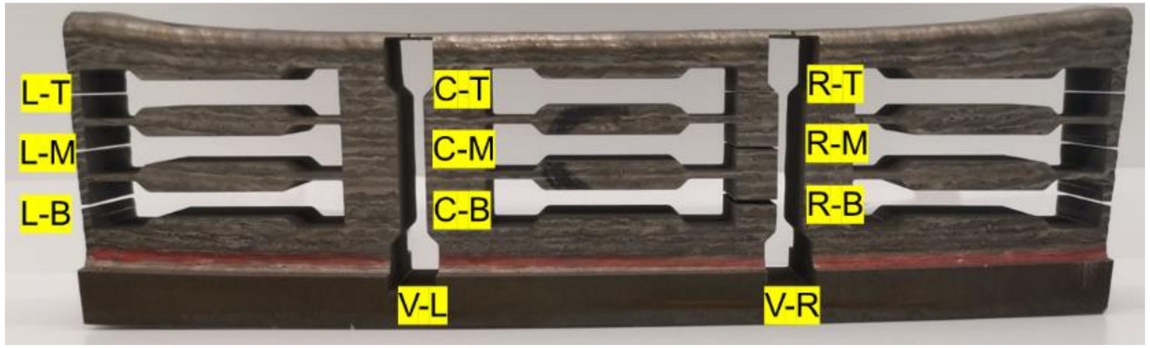
Wall shape sample: Microstructure comparison

As-built condition (different locations)

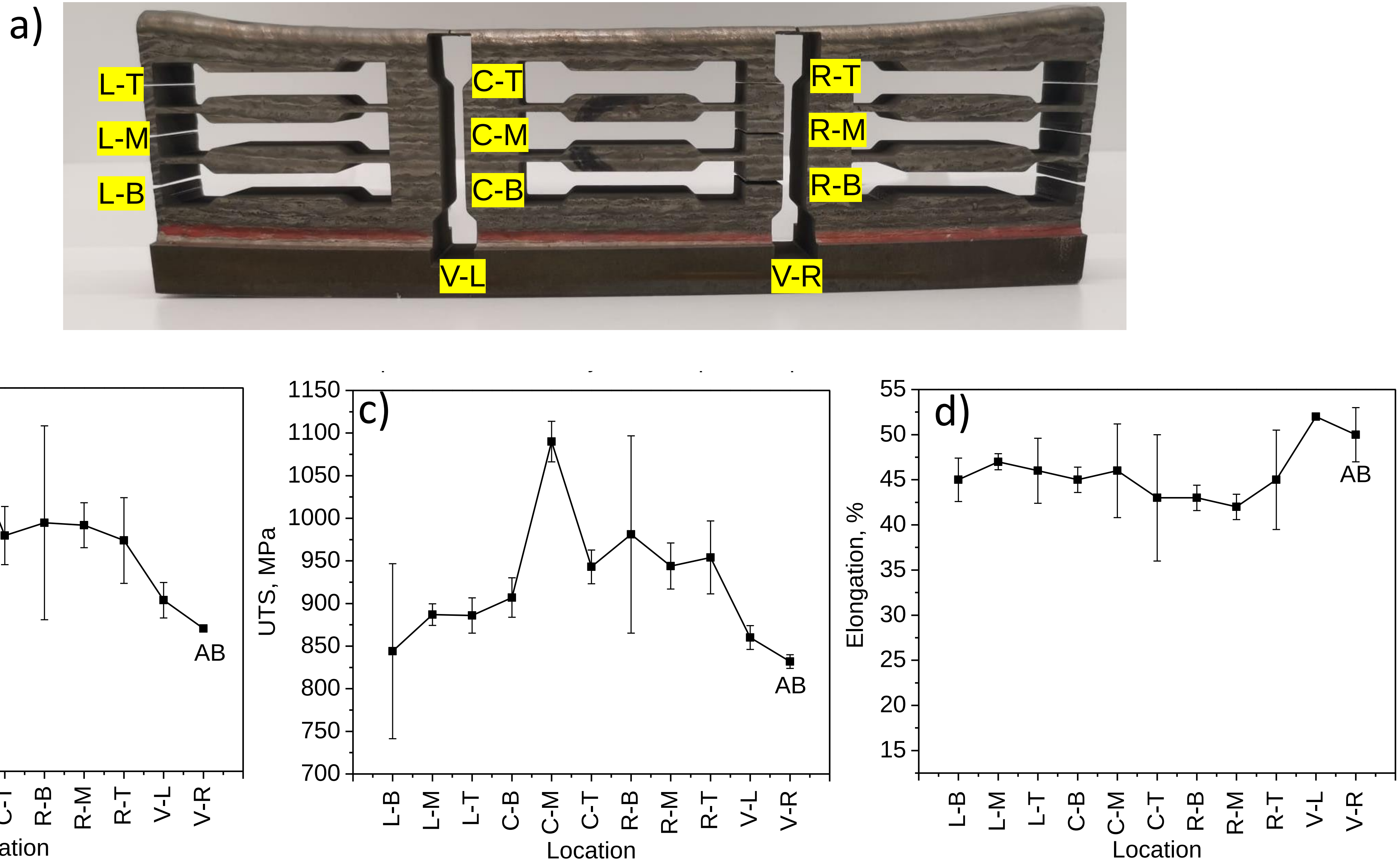


as-built vs. Standard vs. Optimized heat treatment



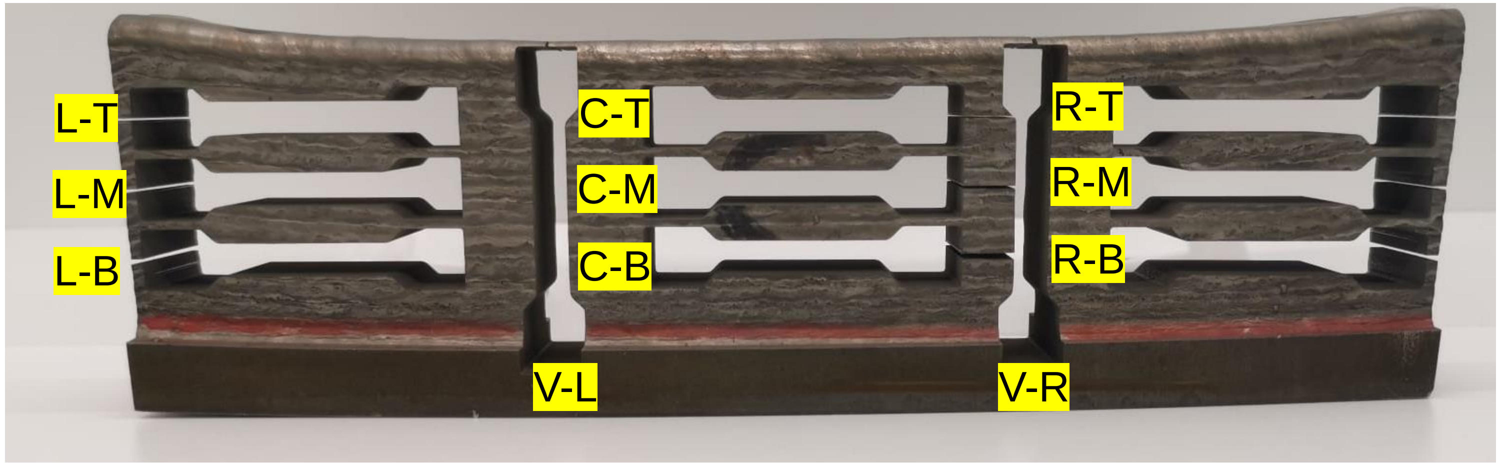


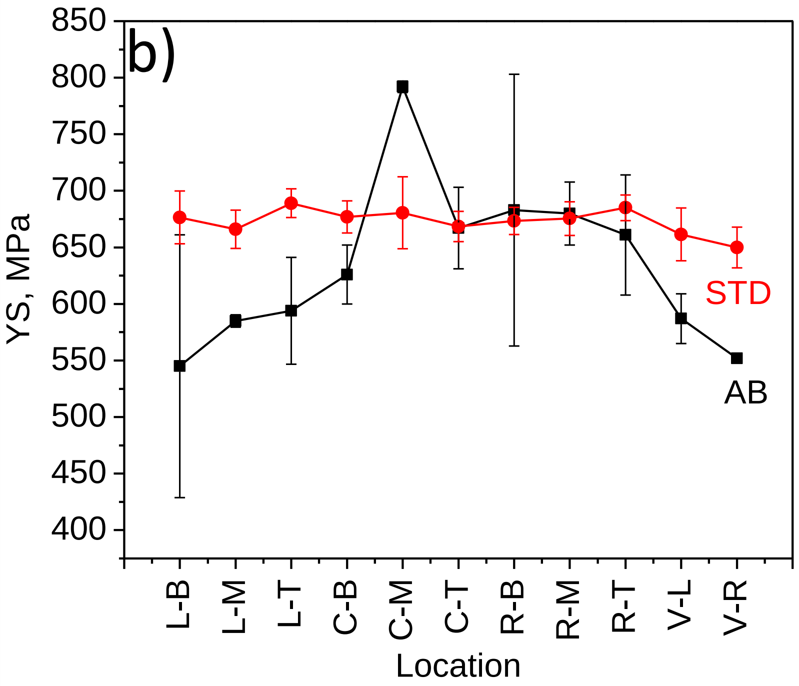
Wall shape sample: Cutting for location specific study

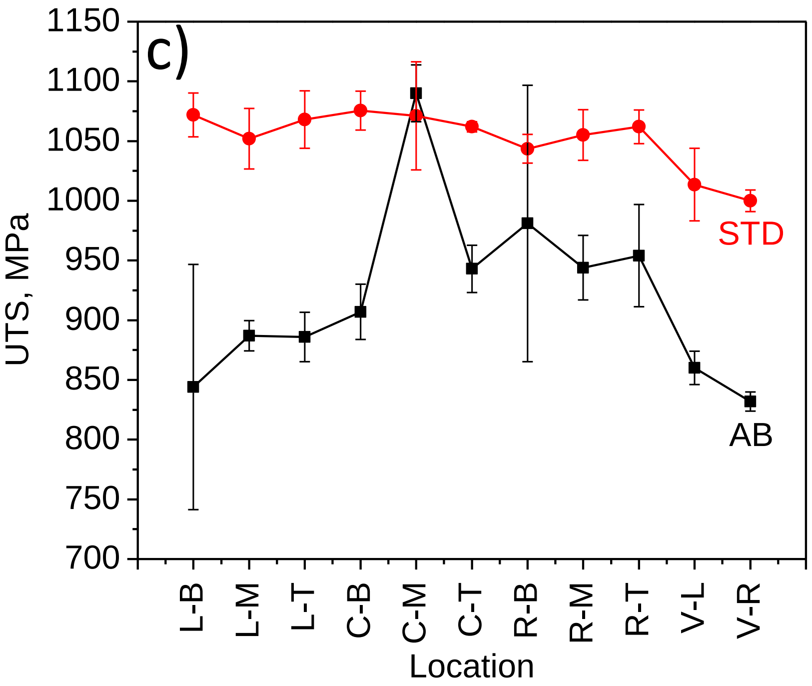


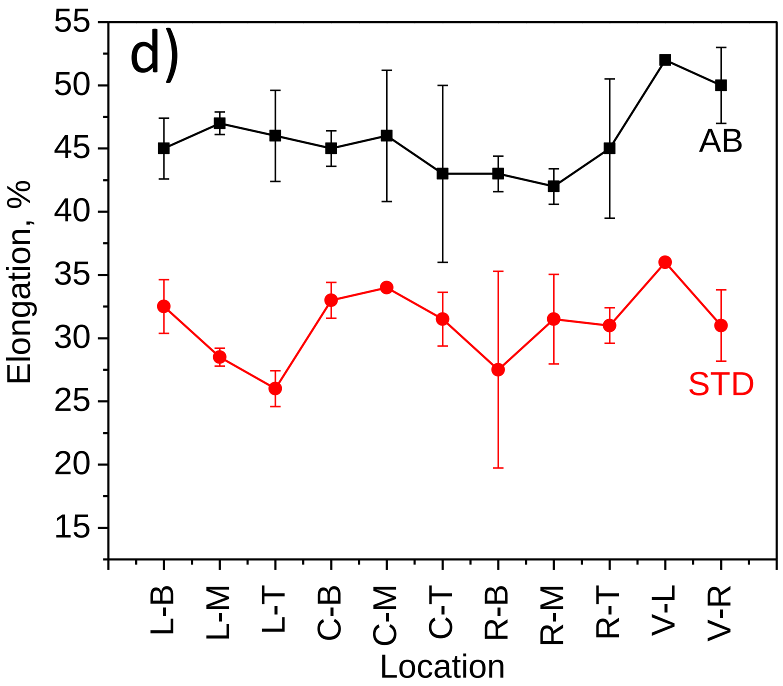
Wall shape sample: Cutting for location specific study

a)



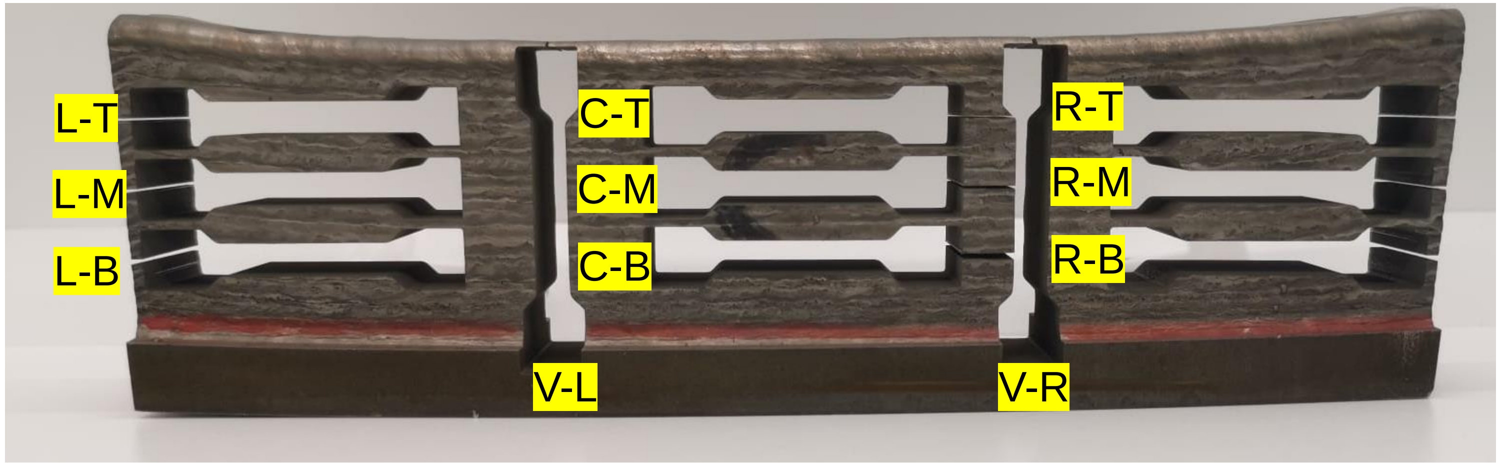


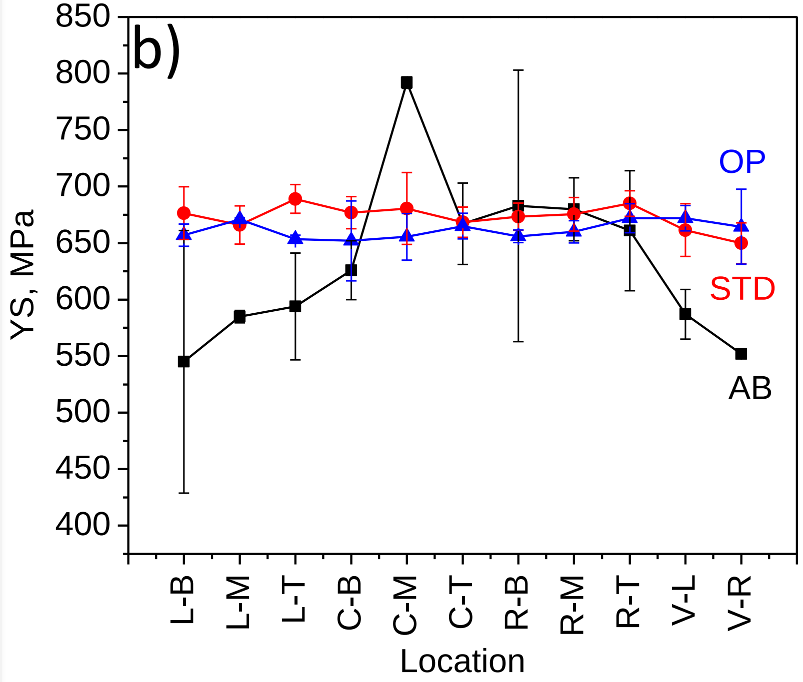


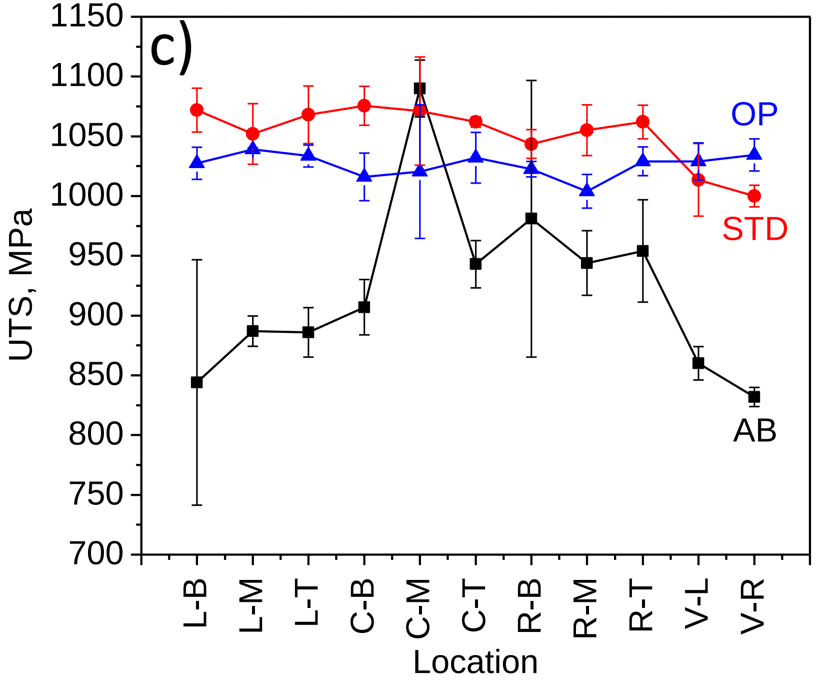


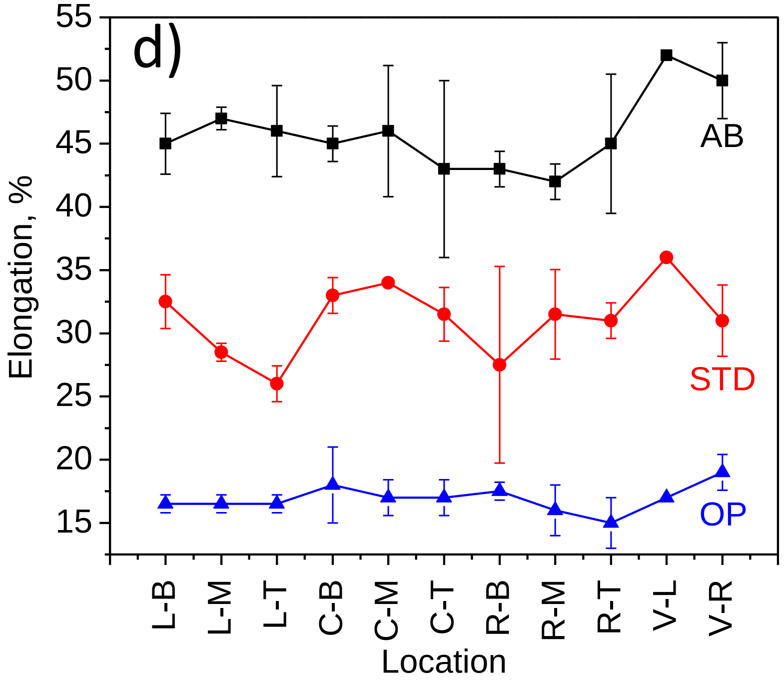
Wall shape sample: Cutting for location specific study

a)







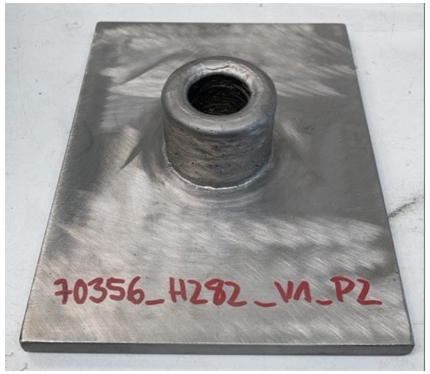


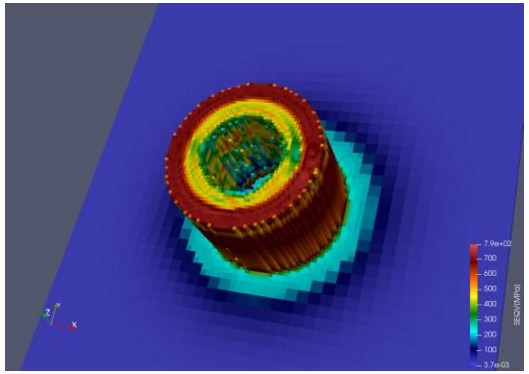
Take-home messages

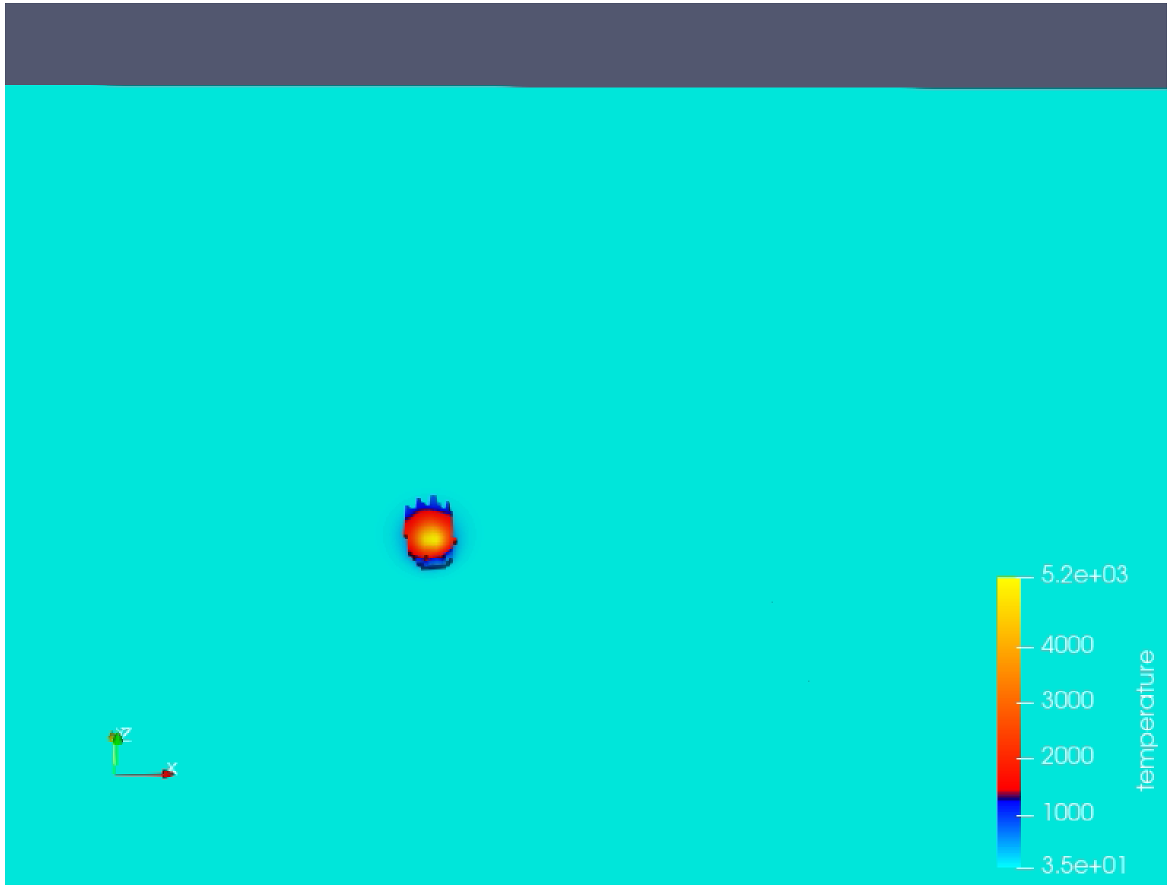
- Recrystallization in WAAM samples can help with grain refinement, however, we should avoid grain boundary melting.
- Recrystallization in WAAM samples is not sufficient enough to introduce small grains.
- CALPHAD-based ICME with enhancement by machine learning is a powerful tool for post-heat treatment design.
- Large sample printed using WAAM is not necessarily show more pronounced heterogeneity in microstructure-property distribution.
- Effective post-heat treatment design can greatly reduce the heterogeneity of microstructure-property distribution.

Physics-based WAAM Process Simulation

- Haynes 282 parameters
- Cylinder of 22 layers
- Mesh size: 500 microns
- Meshing time: 40 min
- Preprocessing time: 15 min
- Simulation time:
  - 2 hours for thermal
  - 29 hours for thermomechanical

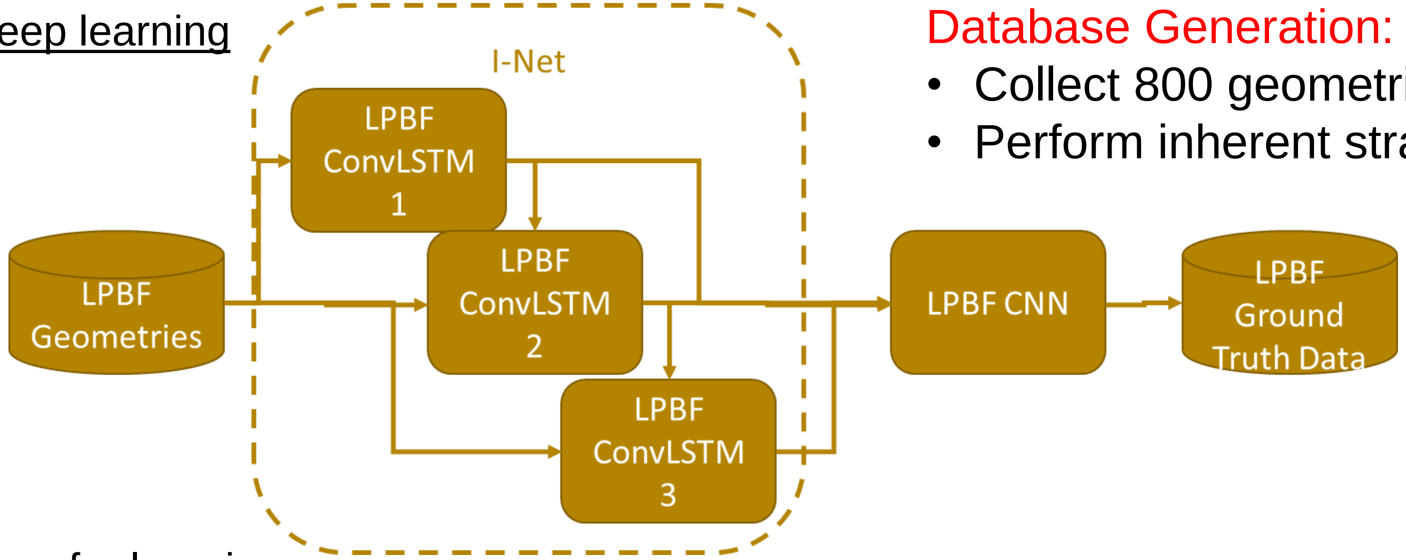






Transfer Learning for Residual Stress Prediction

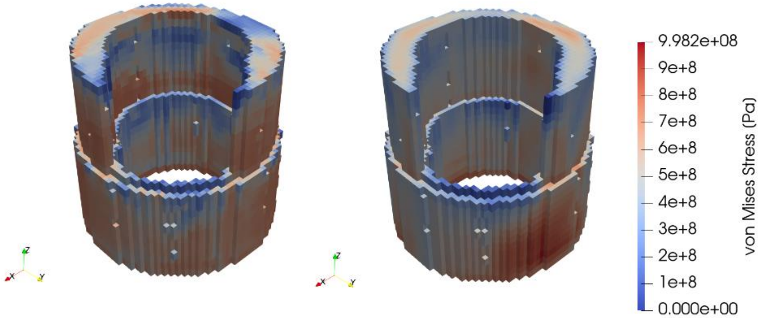
Deep learning



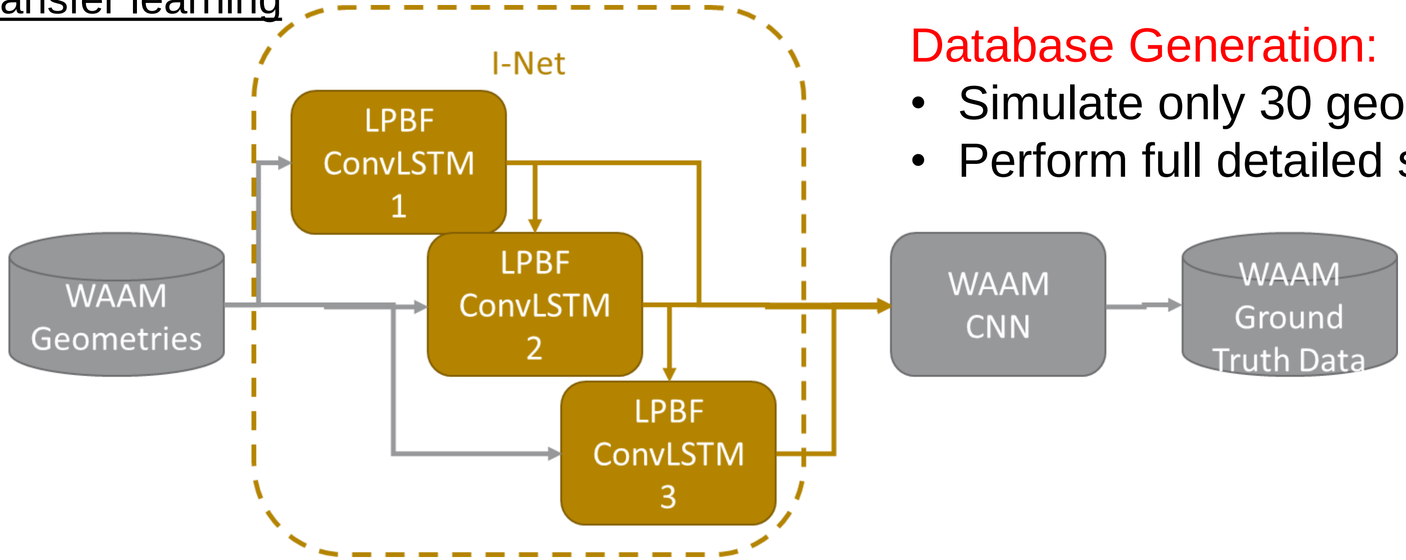
Database Generation:

- Collect 800 geometries
- Perform inherent strain simulation

FEA **Transfer Learning**



Transfer learning



Database Generation:

- Simulate only 30 geometries
- Perform full detailed simulation

Average error: 9%
ML model runtime – < 1 second
Efficiency gain – 10,000x

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☺ *Questions?*
☺ *Suggestions?*