***NETL** Virtual Project Review Meeting, High Performance Materials, 9/22/2020*

Integrated Computational Materials and Mechanical Modeling for Additive Manufacturing of Alloys with Graded Structure used in Fossil Fuel Power Plants

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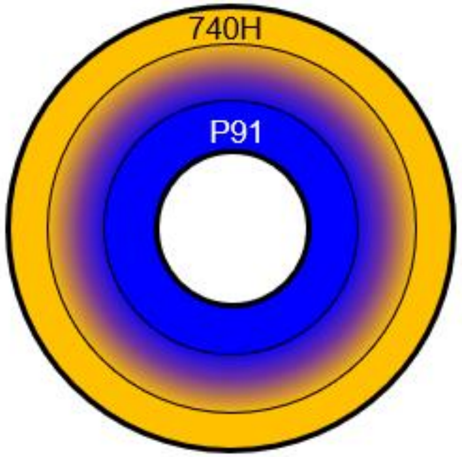
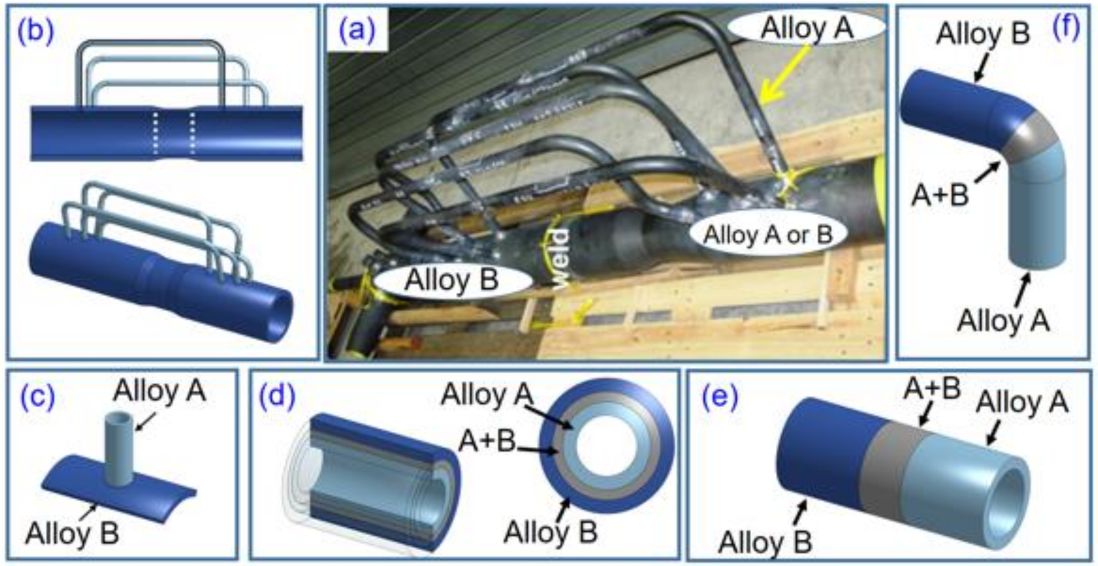
Acknowledgement:

DE-FE0031637

Background and significance

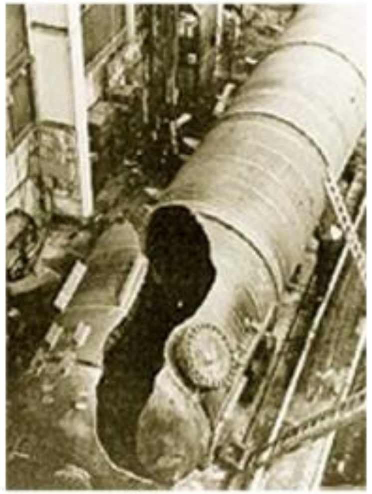
Complex shape manufacturing





Balance between performance and cost

Repair pipeline in a rapid mode

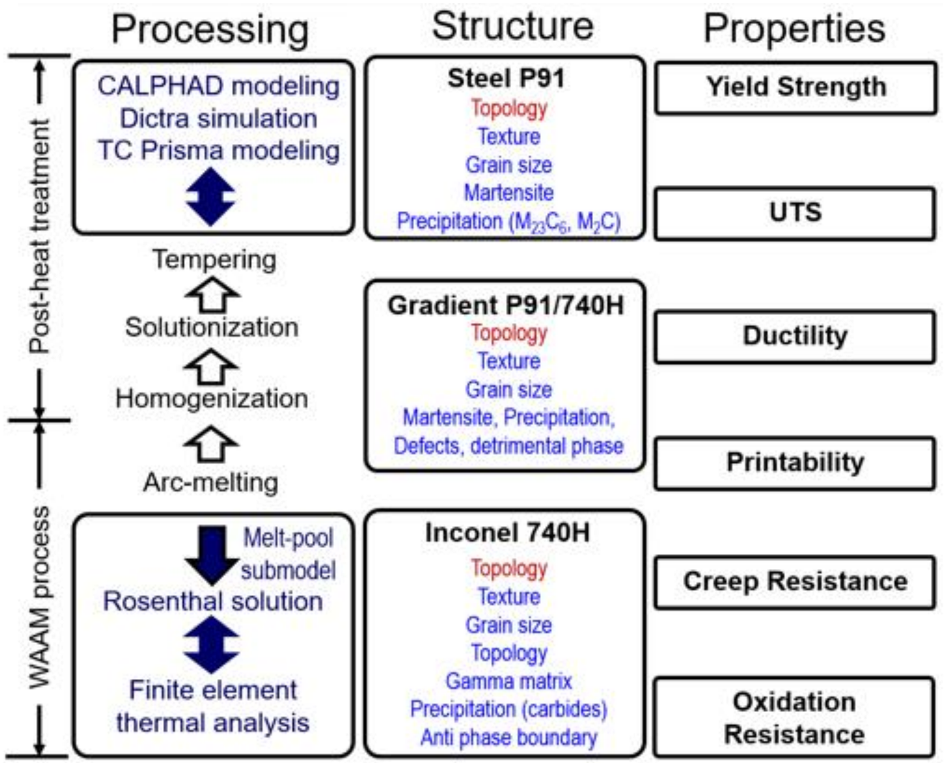


Images from internet

Project objectives

Integrating available computational materials and mechanical engineering **tools for graded structure alloy design** by **WAAM with demonstration.**

1. What are the effective tools can be used for the effective design?
2. What are the limitations of the tools?
3. how to integrate computation and experiments for design purpose?



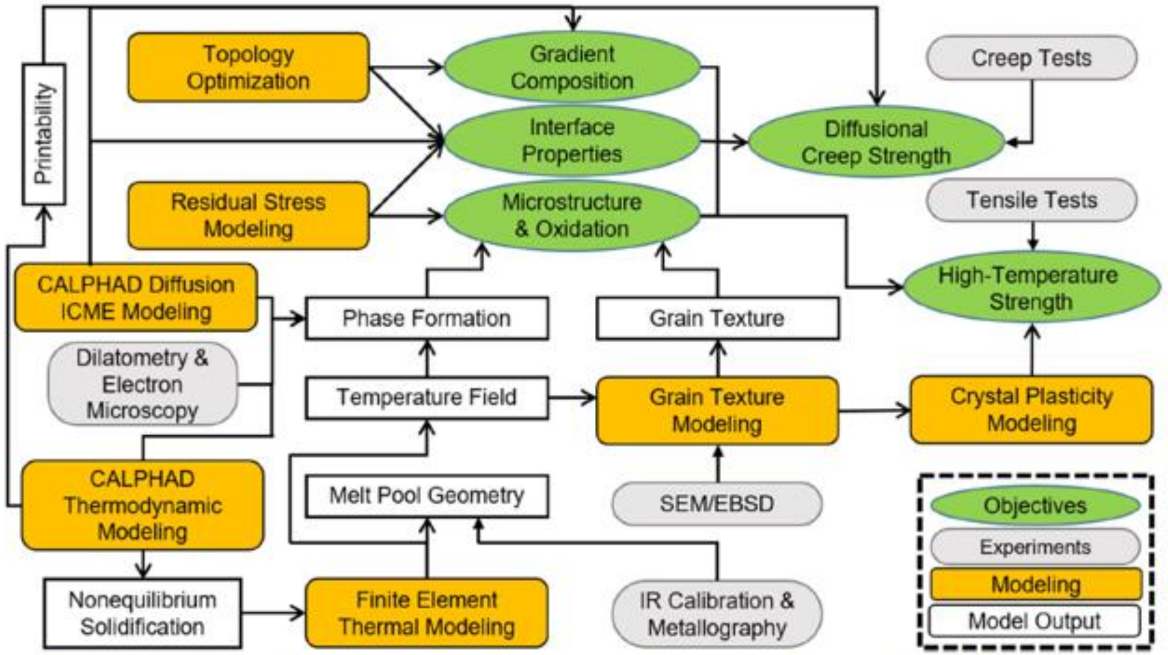
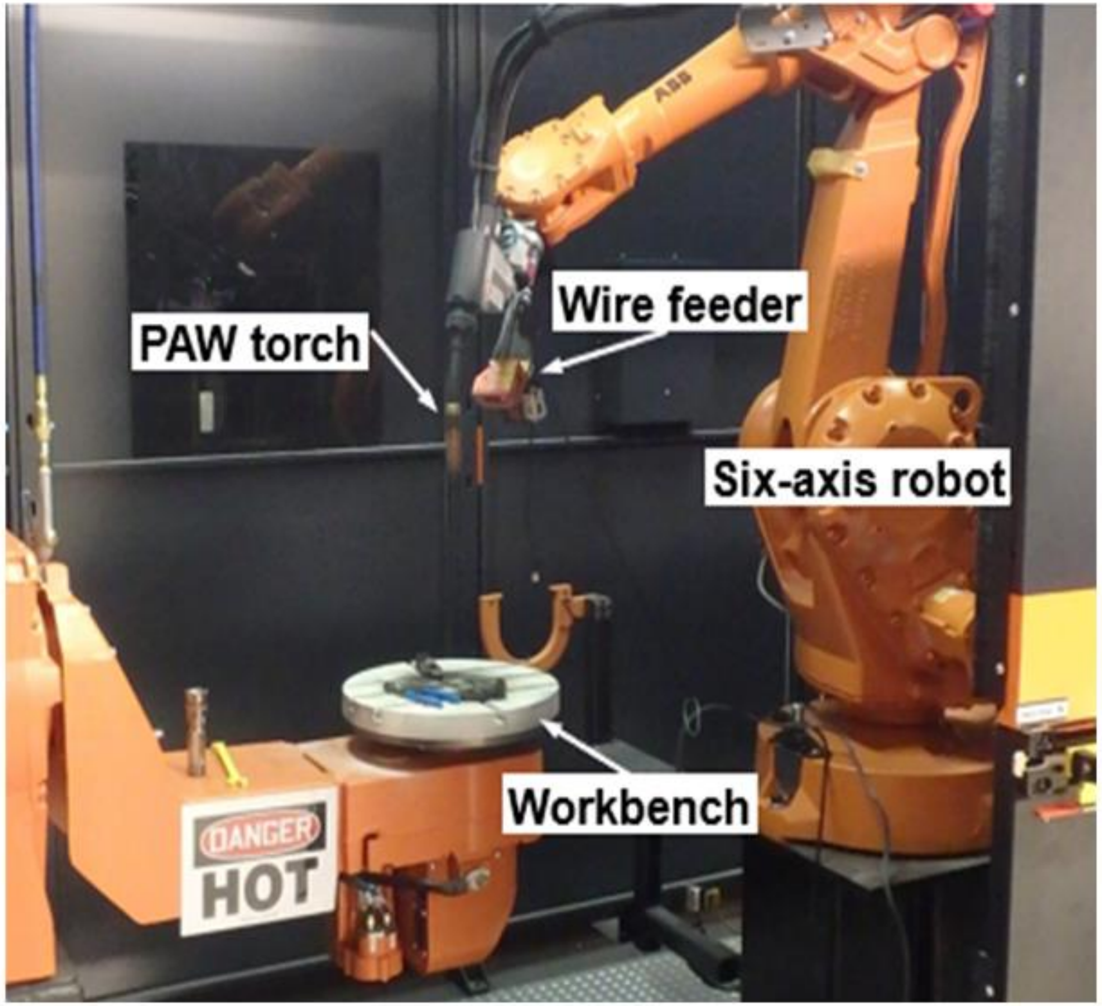


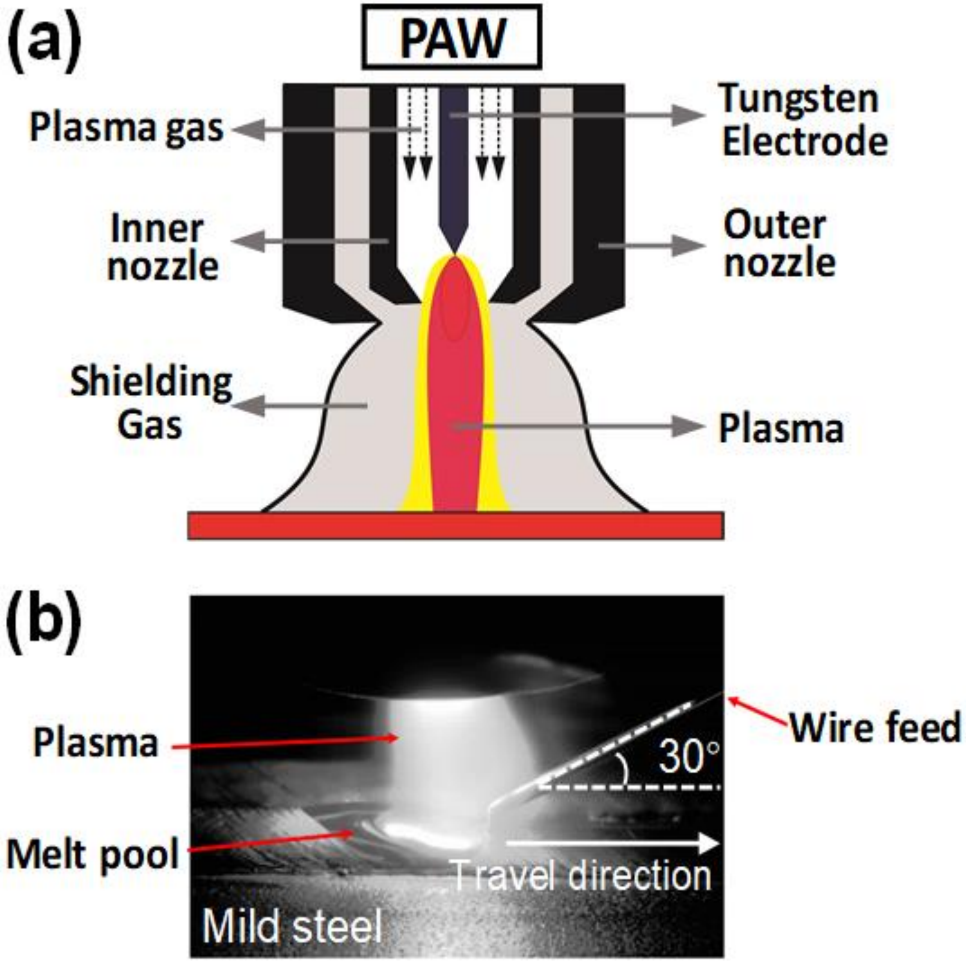
Figure 1. ICME model framework for additive manufacturing of alloys with graded structure.

CALPHAD: Calculation of Phase Diagrams; ICME: Integrated Computational Materials Engineering

WAAM setup

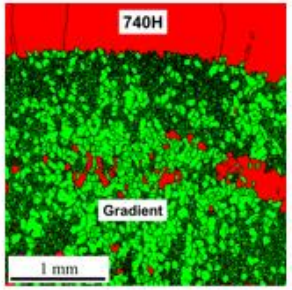


WAAM setup available in RTRC showing the PAW torch, 6-axis robot and wire feeder



(a) Schematic of the PAW torch and (b) in-situ observation during the deposition

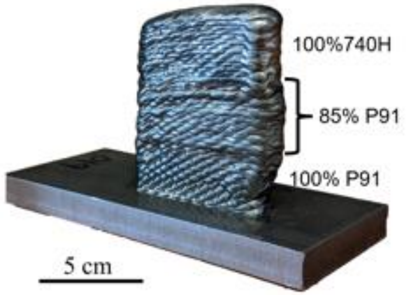
Design Strategy

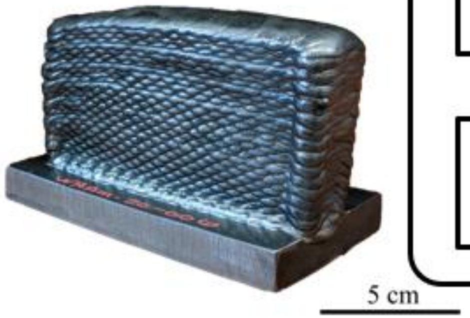


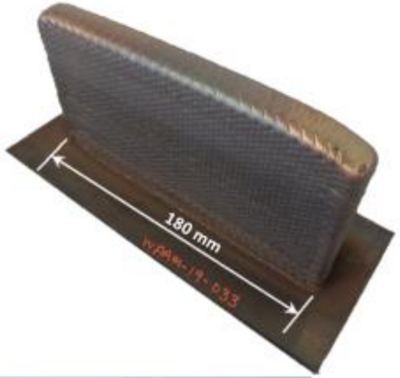
Design of Gradient Microstructure + Design of Gradient Interface Structure

↑ Post-heat treatment of 740H by WAAM ← WAAM of 740H (single build)

↑ Post-heat treatment of P91 by WAAM ← WAAM of P91 (single build)







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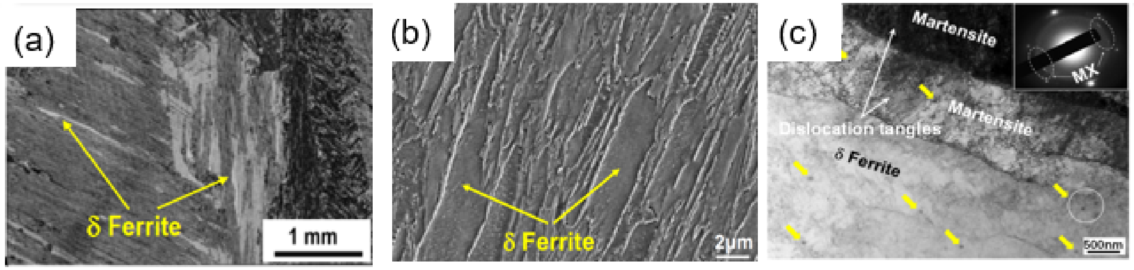
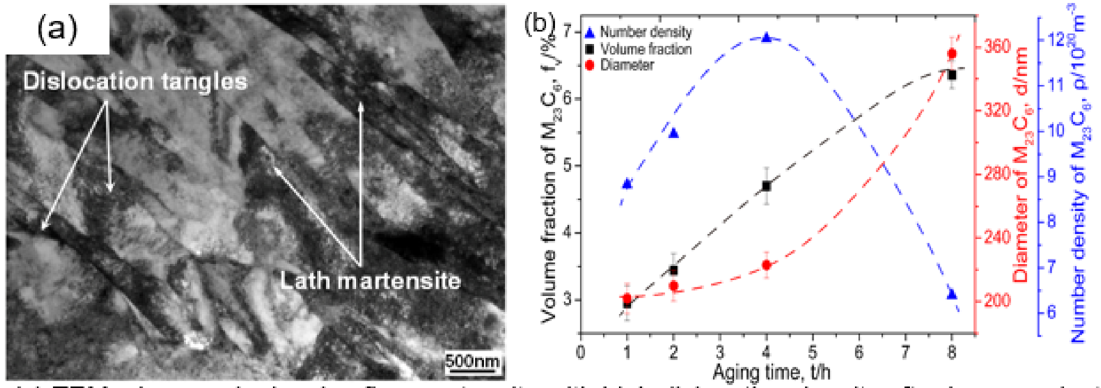
P91 and 740H single component builds

K, Li, M. Klecka, S. Chen, W. Xiong,
Additive manufacturing, under revision



(a) Optical, (b) SEM and (c) TEM images of as-built P91 steel showing the presence of δ-ferrite

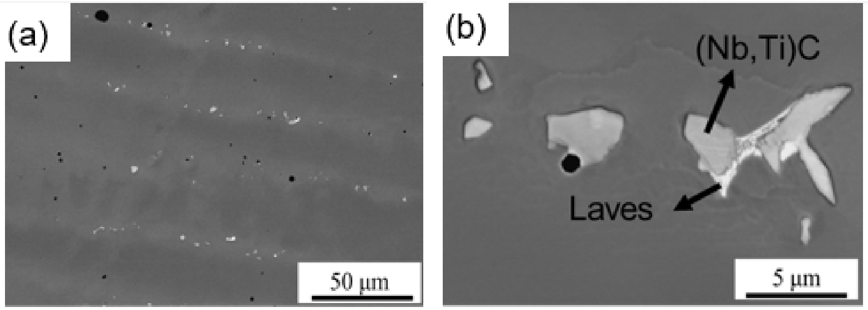


(a) TEM micrograph showing fine martensite with high dislocation density after homogenization for 2 hrs at 1200°C and (b) precipitate evolution after at 760°C showing that 2 hrs is the optimum

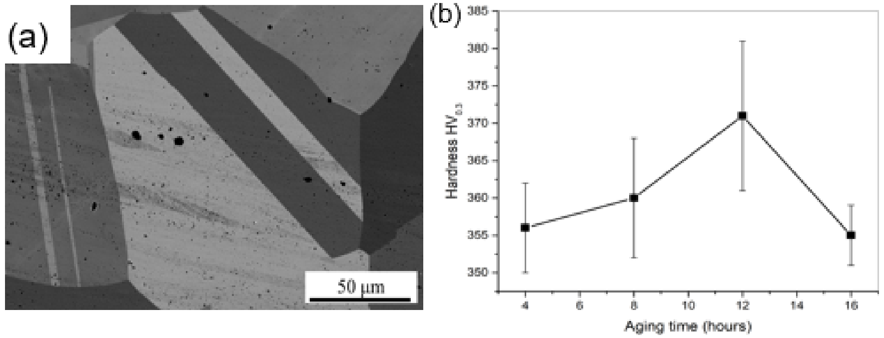
Optimum post-heat treatment for WAAM P91:
Homogenization at 1200°C for 2 hrs and aging at 760°C for 2 hrs

Tensile properties of P91 steel at different conditions

	YS (MPa)	UTS (MPa)	Elongation (%)
As-built	985	1242	10.9
Aged	686	774	19.4
Wrought	415	585	20



BSE-SEM images showing the presence of Laves and MC carbides in as-built 740H



(a) BSE-SEM image showing dissolution of Laves and annealing twins after homogenization at 1200°C for 2 hrs and (b) peak hardness at 760°C for 12 hrs.

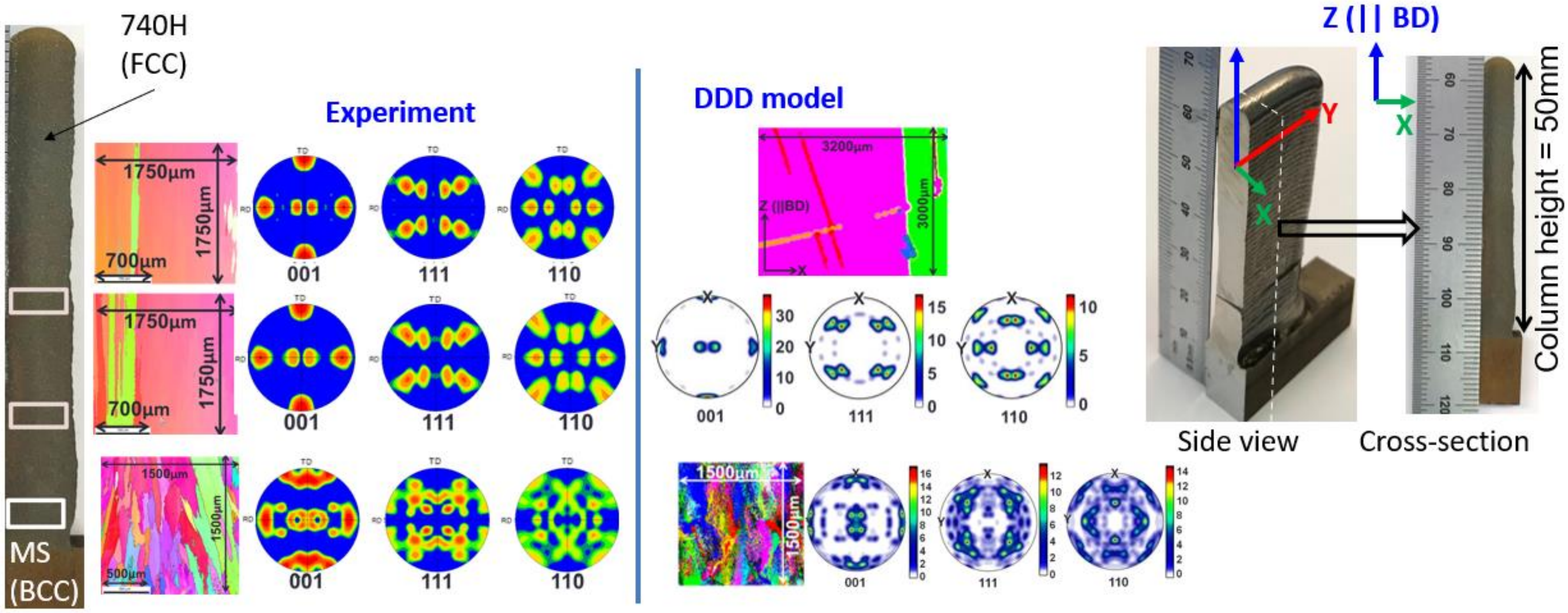
Optimum post-heat treatment for WAAM 740H:
Homogenization at 1200°C for 2 hrs and aging at 760°C for 12 hrs

Tensile properties of 740H superalloy at different conditions

	YS (MPa)	UTS (MPa)	Elongation (%)
As-built	649±19	925±14	37.5±2.4
Aged	655±18	963±11	29.5±1.2
Target	620	--	23

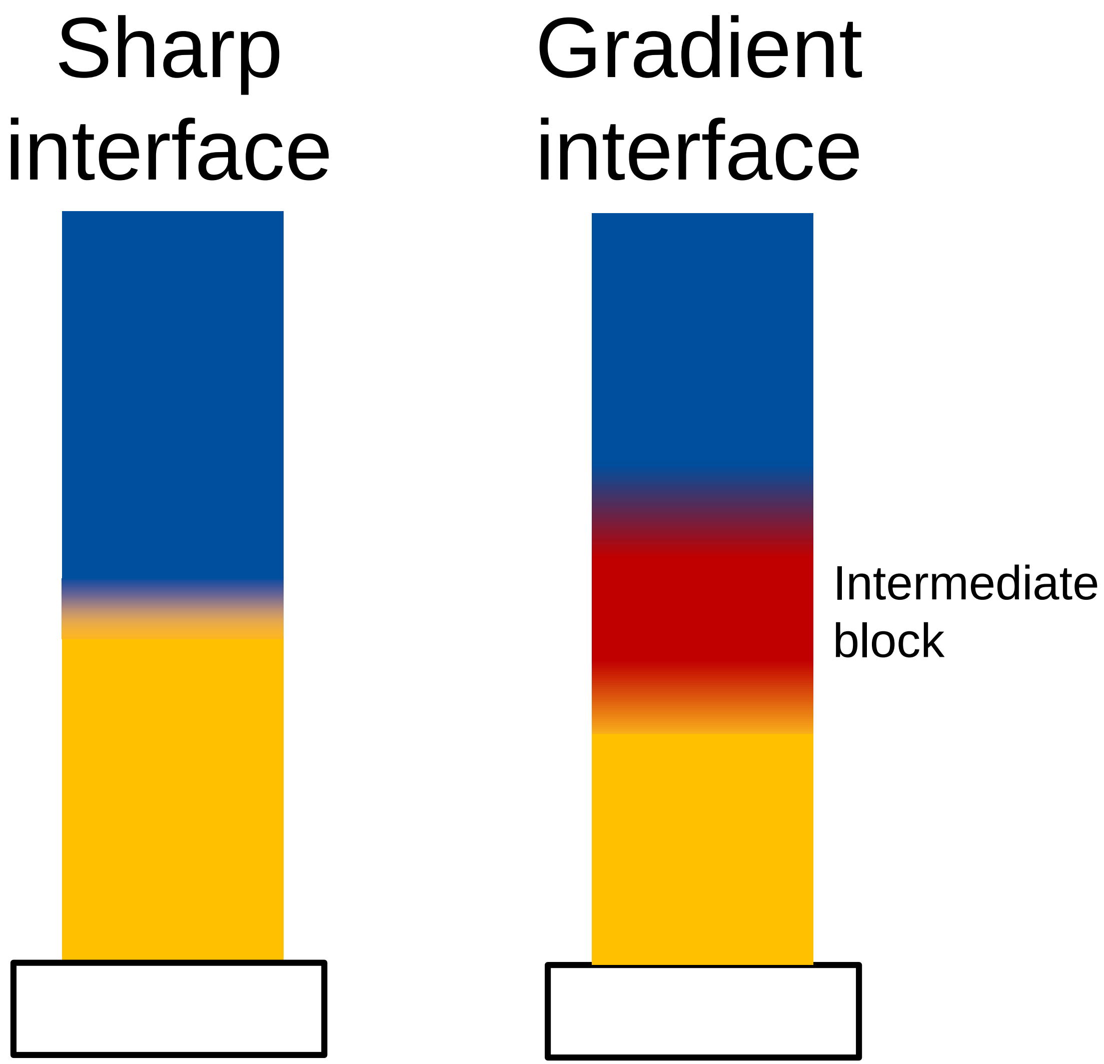
Grain texture prediction for 740H using Discrete Dendrite Dynamics

Paul, S., Liu, J., Zhao, Y., Sridar, S., Klecka, M., Xiong, W., To, A., *A Discrete Dendrite Dynamics Model for Epitaxial Columnar Grain Growth in Metal Additive Manufacturing with Application to Inconel*. ***Additive Manufacturing*** **(accepted for publication), 2020**



DDD model predicts the microstructure of entire WAAM processed 740H superalloy build successfully

Sharp interface builds



Sharp interface gradient builds (P91 on 740H vs. 740H on P91)

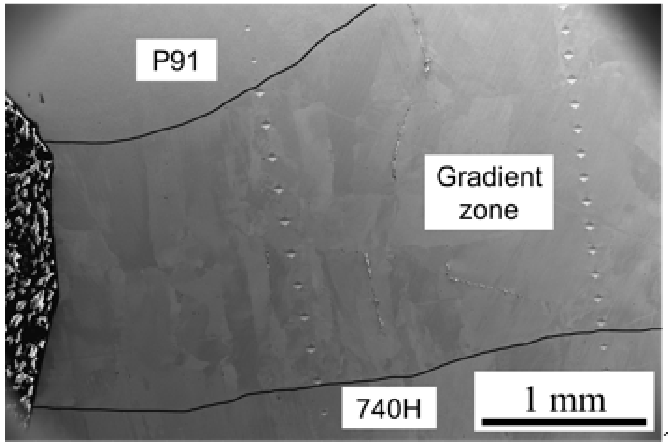
Deposition of 15 layers of P91 steel (interpass cooling = 1 minute)

↑

Cooling time = 20 minutes

↑

Deposition of 15 layers of Inconel 740H (interpass cooling = 1 minute)



Printing strategy used and BSE-SEM micrograph showing large gradient zone in direct deposition of P91 over 740H (740H/P91).

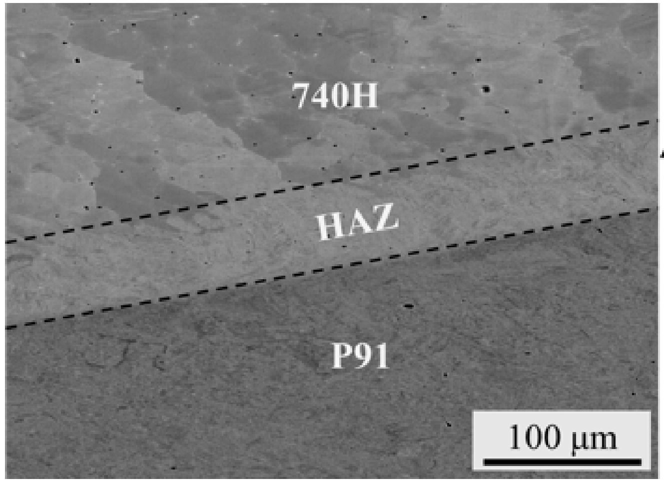
Deposition of 15 layers of Inconel 740H (interpass cooling = 1 minute)

↑

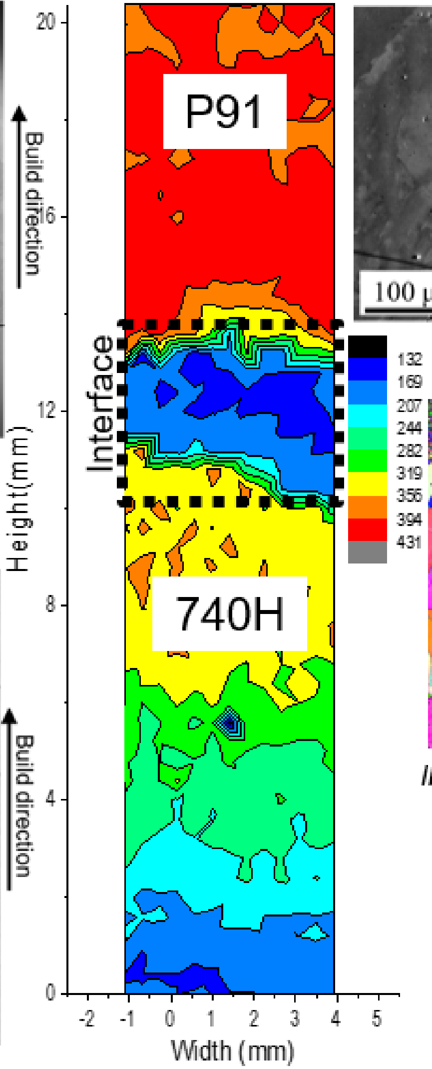
Cooling time = 120 minutes

↑

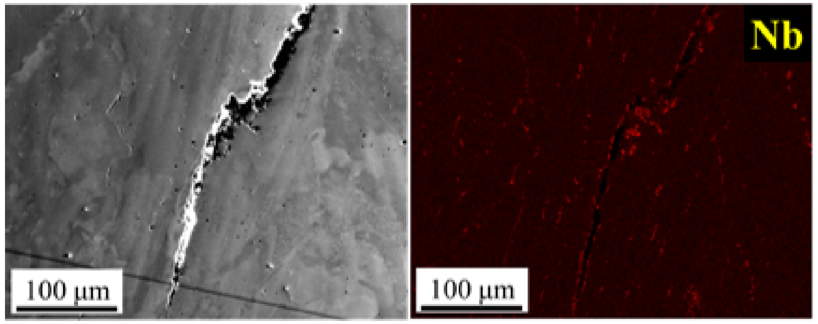
Deposition of 15 layers of P91 steel (interpass cooling = 1 minute)



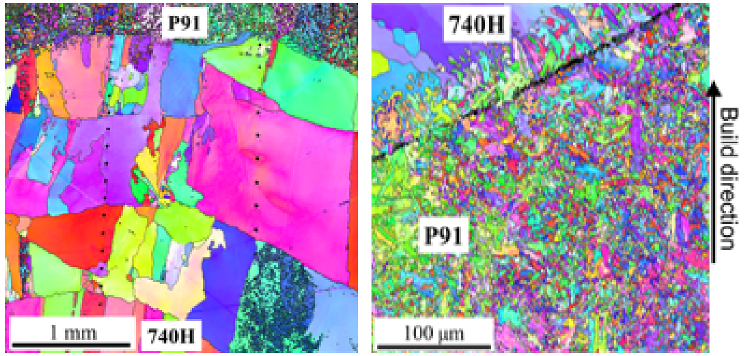
Printing strategy used and BSE-SEM micrograph showing thin gradient zone in direct deposition of 740H over P91 (P91/740H).



Hardness map along build direction for 740H/P91 showing a gradient zone with low hardness



SEM micrograph of the crack and composition map obtained by EDS for 740H/P91.



IPF maps showing the coarse grains in gradient zone of 740H/P91 and fine grained HAZ in P91/740H

Deposition of 740H over P91 is the desirable sequence since there were

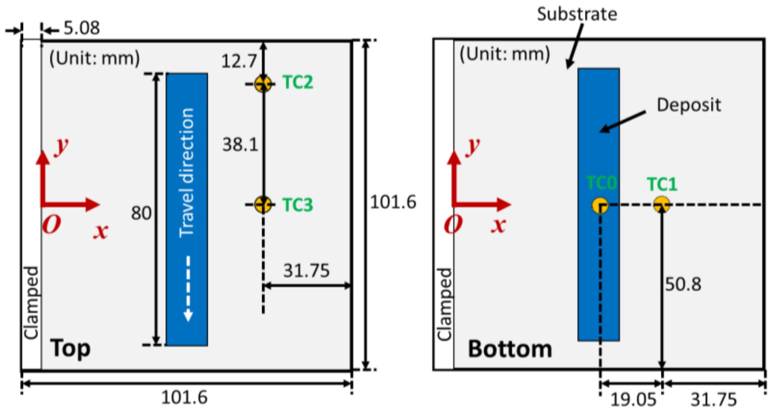
- *No defects in the interface*
- *No deleterious phases formed*

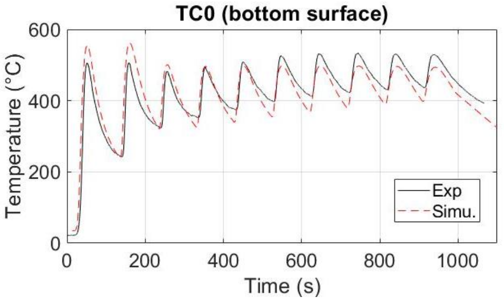
Thermal modeling and residual stress modeling

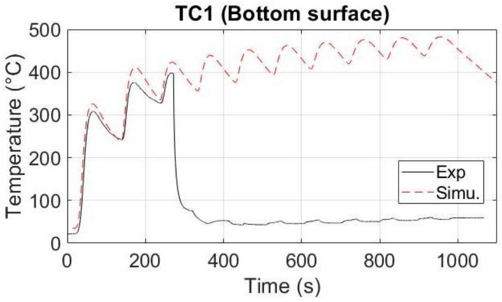
The model was calibrated using 10 layers, single track for single component builds

Thermal model

Calibrated using thermocouple and melt pool measurements

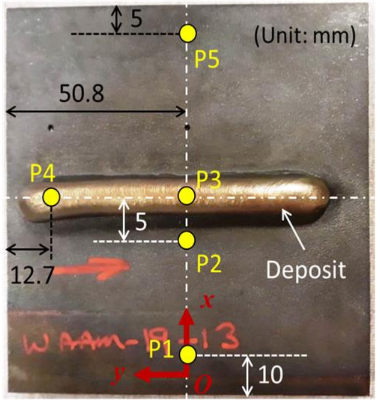






Mechanical Model

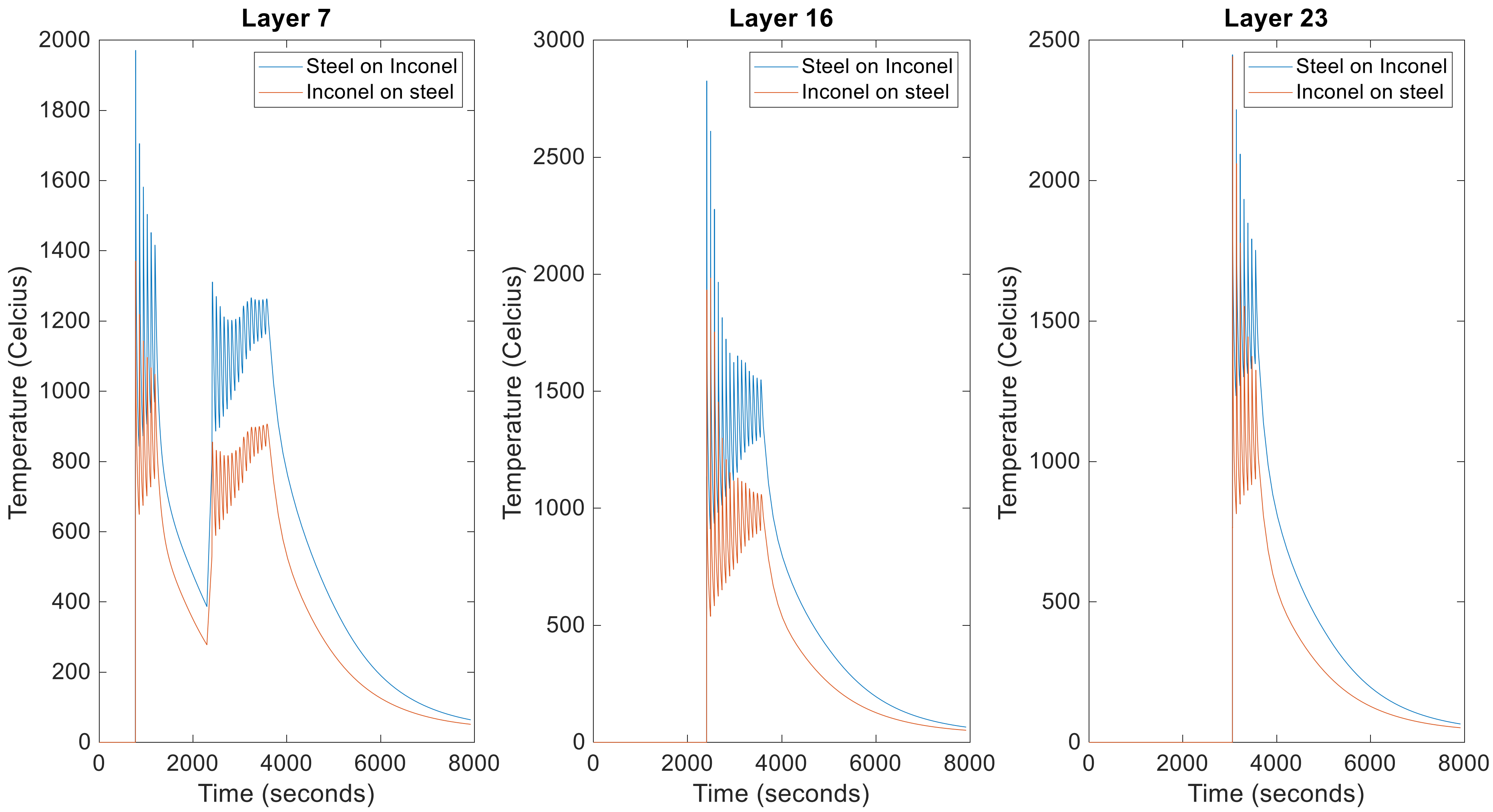
Validated using X-ray diffraction



Location	Index	XRD (MPa)	Simulation w/o phase transformation		Simulation w/ phase transformation	
			Residual stress (MPa)	Error with XRD	Residual stress (MPa)	Error with XRD
Substrate (A36)	P1	52 ± 5	81	+55.8%	62	+19.2%
	P2	216 ± 7	190	-12.6%	220	+1.9%
	P5	50 ± 3	219	+338.0%	116	+132.0%
Deposit (B91)	P3	118 ± 44	400	+239.0%	140	+18%
	P4	124 ± 50	181	-46.0%	150	+21.0%

Thermal results

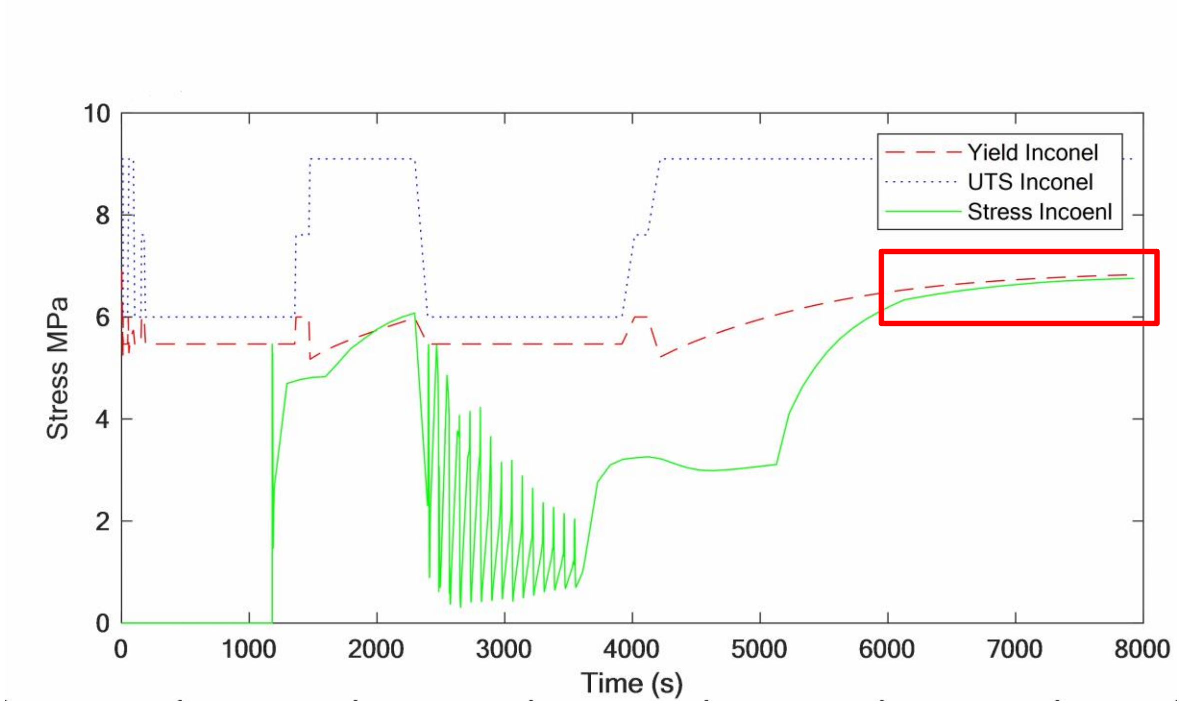
Thermal Conductivity of IN740H is ~2x smaller than P91



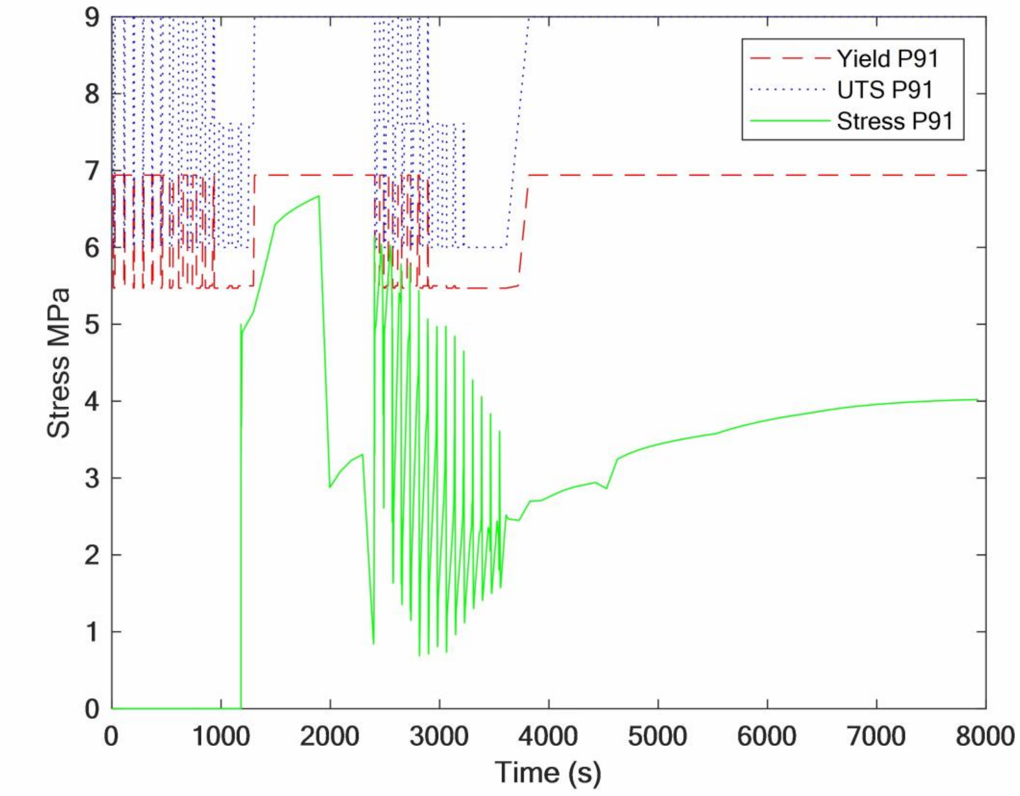
Temperature drop is much higher in the “Steel on Inconel” than in “Inconel on Steel” → perhaps a key reason of cracking in the former case

Residual Stress Simulation

Steel P91 over Inconel 740H

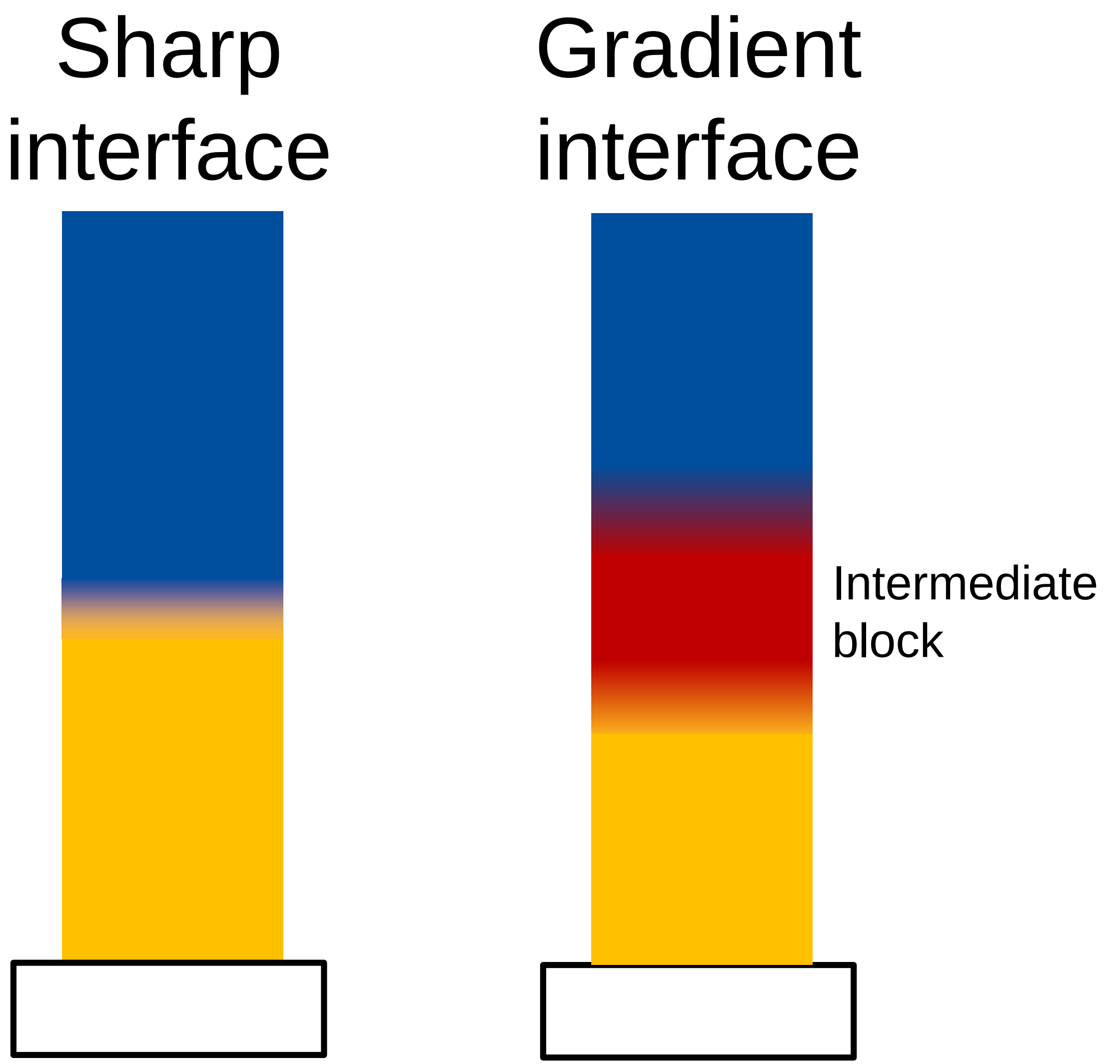


Inconel 740H over Steel P91

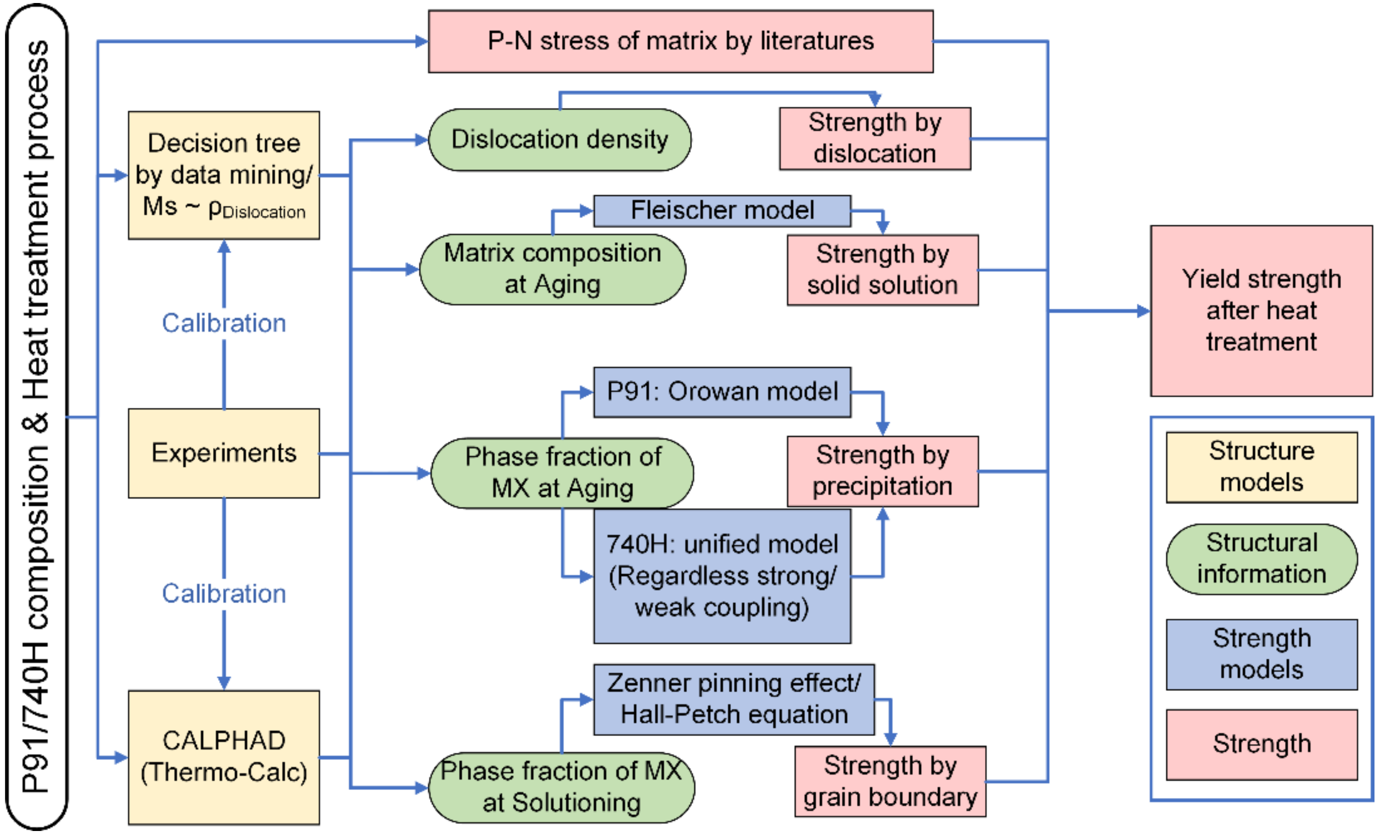


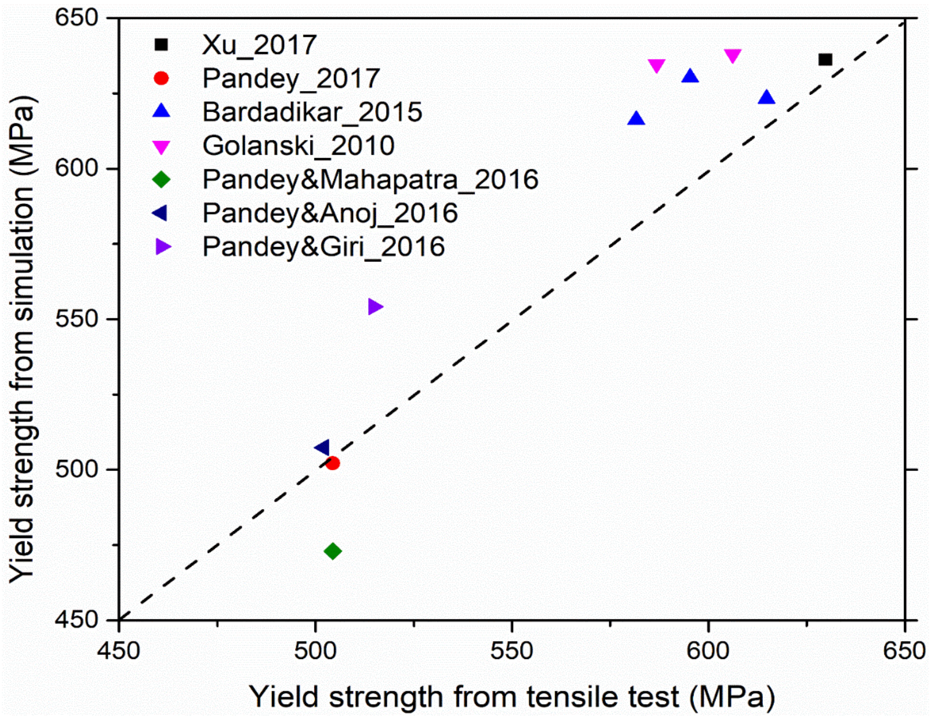
Residual stress much higher in the “Steel over Inconel” simulation case

Gradient interface builds



Structure-property modeling: yield strength modeling





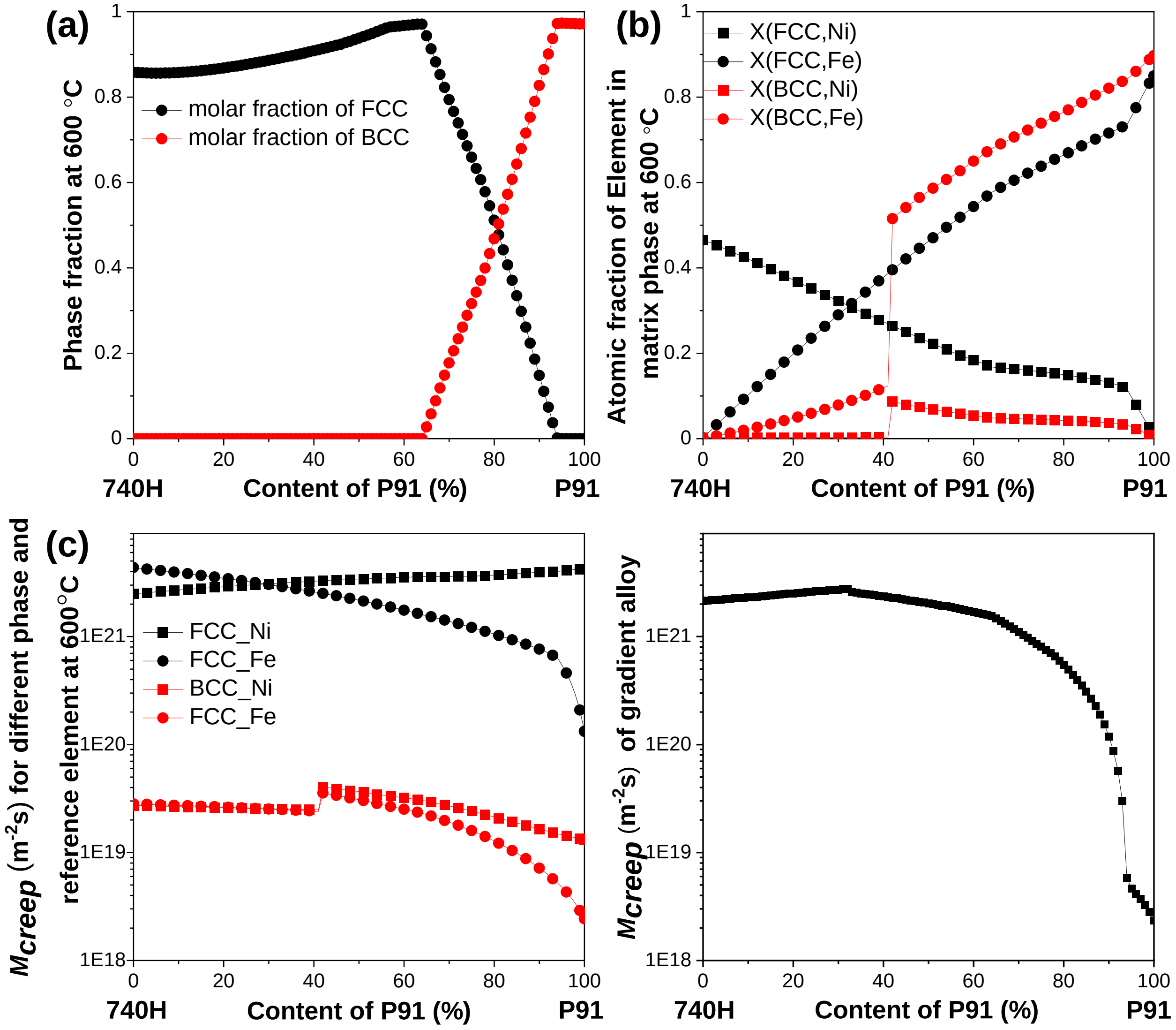
Structure-property modeling: creep design modeling

Creep merit index, M^{creep}:

$$M^{creep} \propto \sum_i^n \frac{x_i}{\exp(-\frac{Q_i}{RT})} \propto \sum_i^n \frac{x_i}{\exp(-\frac{\widetilde{Q_i}}{RT})} \propto \sum_i^n \frac{x_i}{\widetilde{D_i}}$$

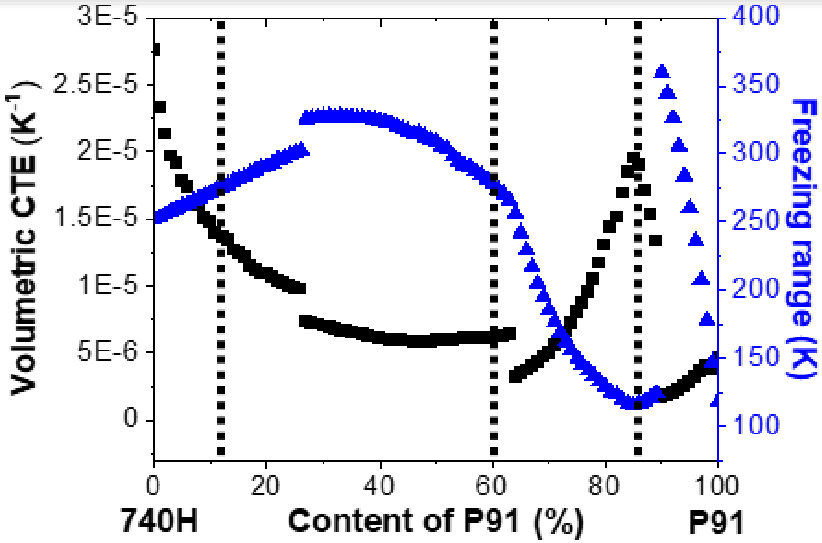
$$M_{alloy}^{creep} = M_{bcc}^{creep} \cdot x_{bcc} + M_{Fcc}^{creep} \cdot x_{fcc}$$

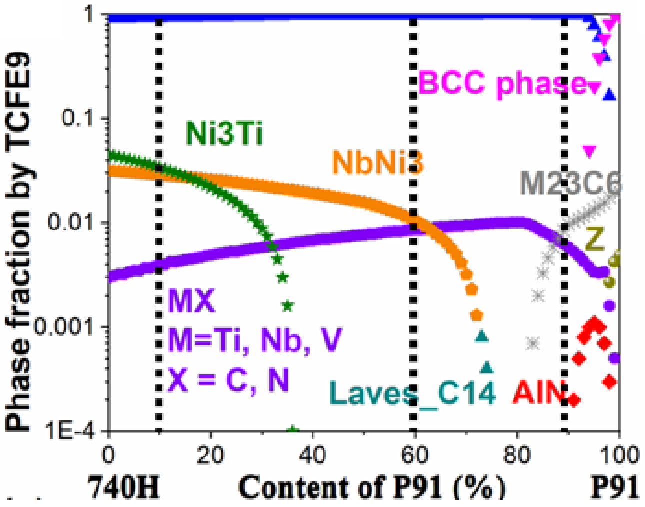
Diffusional creep is considered in this design model framework.
Only tendency variation is predicted.

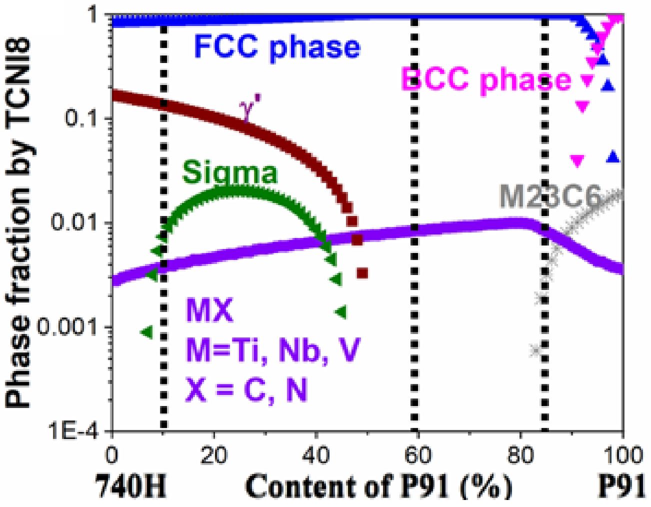


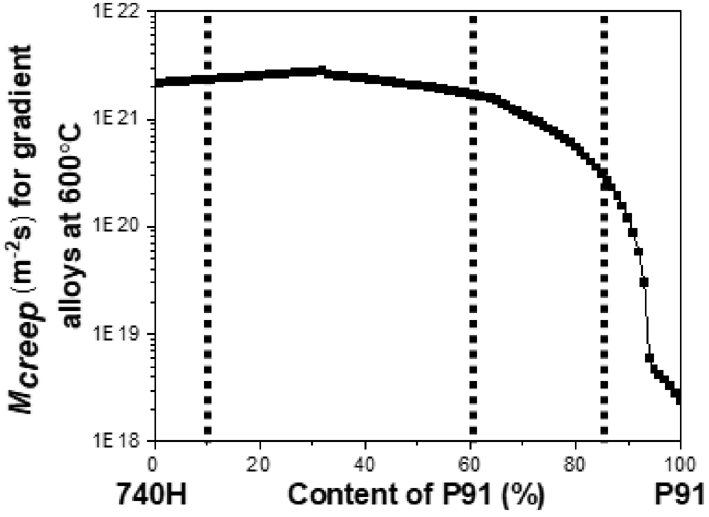
Reed, R. C., T. Tao, and N. Warnken. *Acta Materialia* 57.19 (2009): 5898-5913.

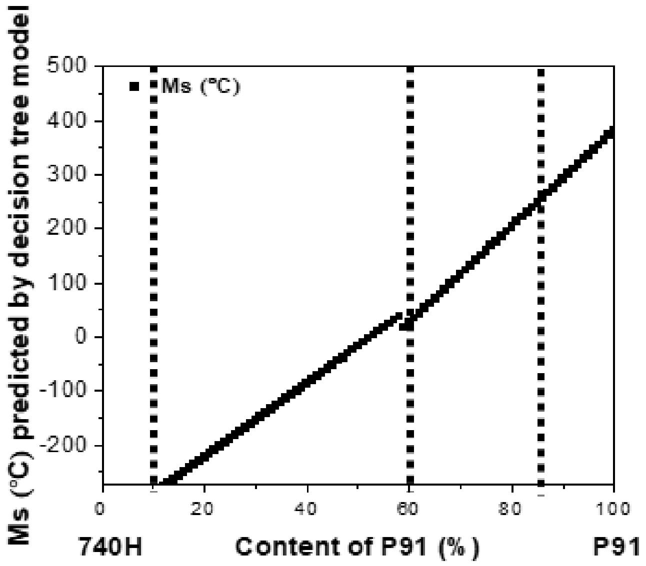
Composition design modeling for graded alloy builds





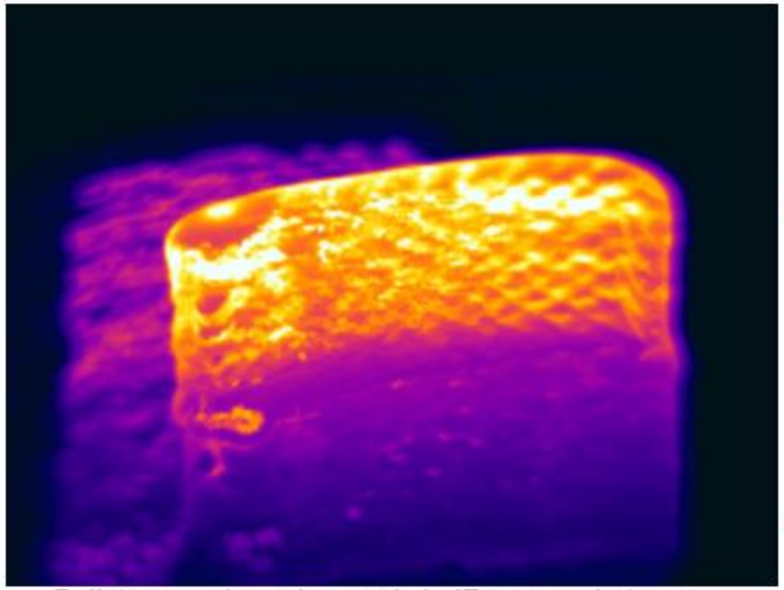




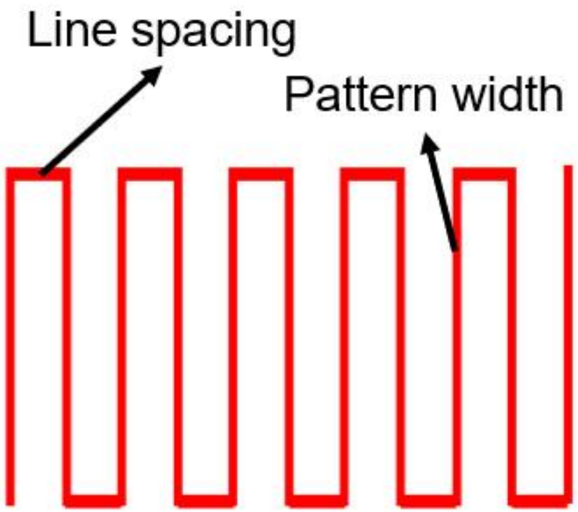


WAAM of gradient builds with graded interface

In-situ observation of the twin-wire feed during deposition



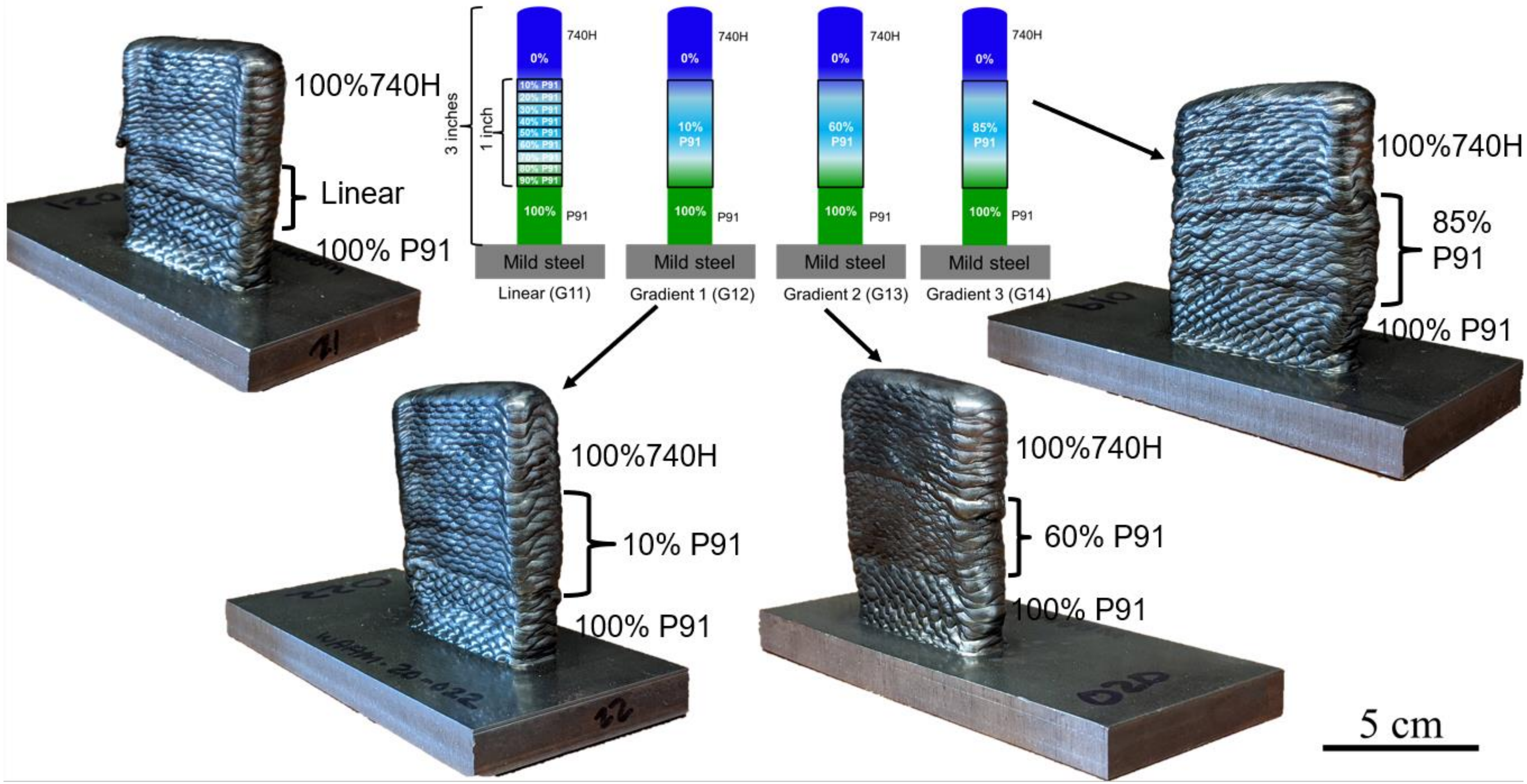
Bulk temperature observed via IR camera between deposited layers. The upper layers (740H) have much lower thermal conductivity and take longer time to cool.



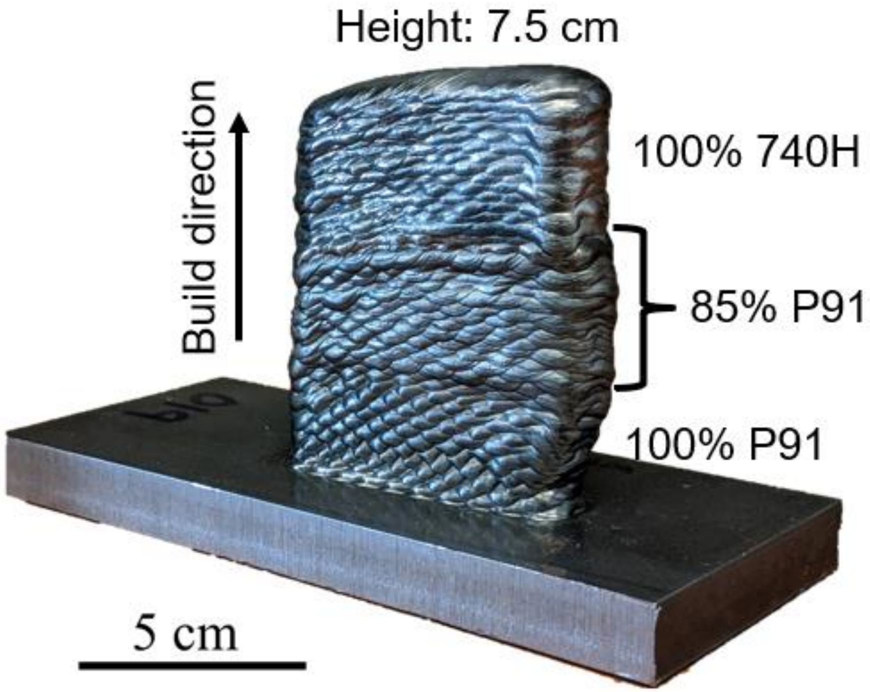
Toolpath used for gradient deposition

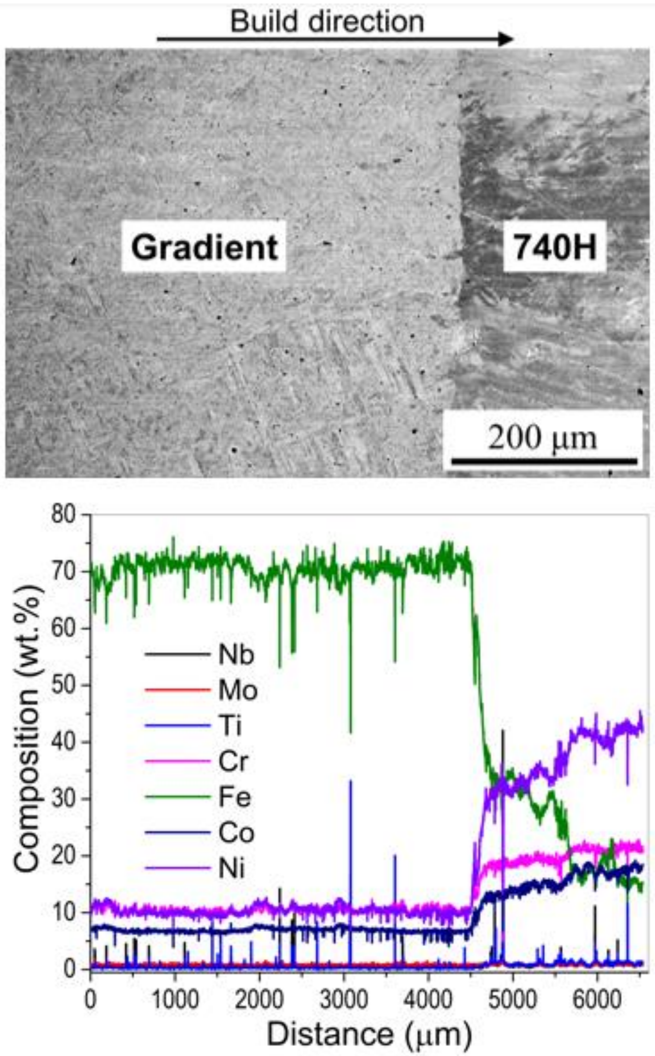
- IR camera used to observe bulk coupon temperature between deposit layers
- Interpass temperature maintained to be below 175°C prior to depositing next layer to avoid diffusion or dilution between layers
- Individual wire feed rates were specified for alloy blending
- Base layers deposited at slightly higher power, to encourage good fusion to substrate
- Overall mass deposition rate is approximately 2 lb/hr which is similar to the previous sharp interface and single component builds

Gradient build with gradient interface fabricated using WAAM

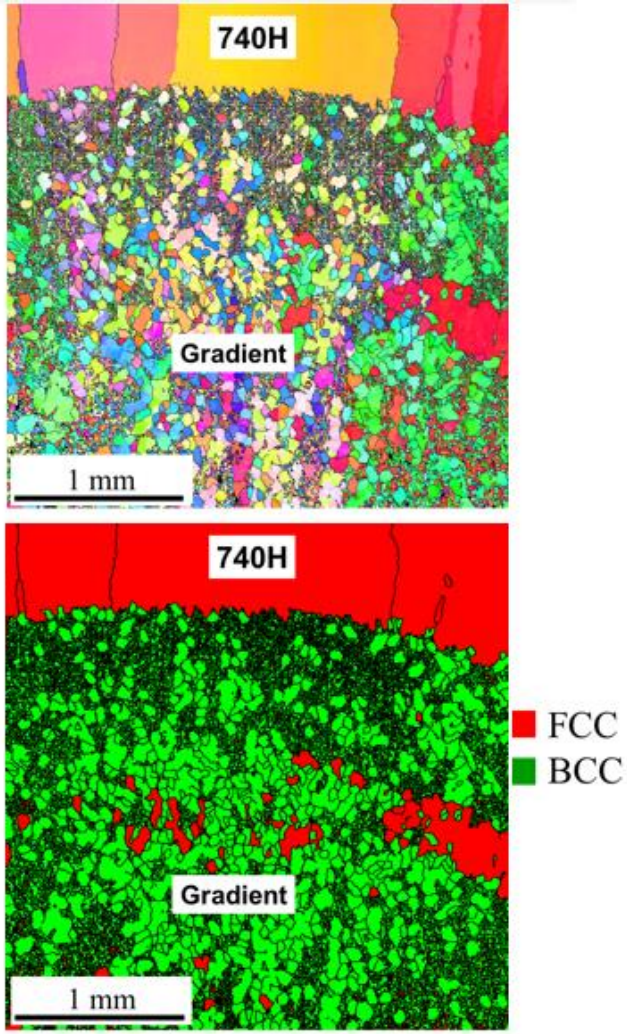


Gradient build with 85% P91 steel interface



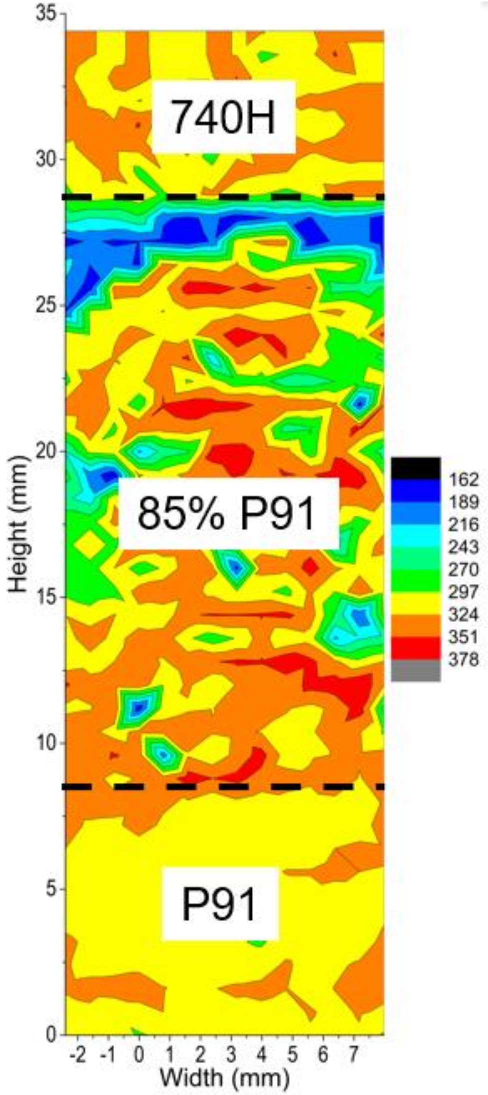


BSE-SEM image and composition profile from EDS across the interface between gradient and 740H

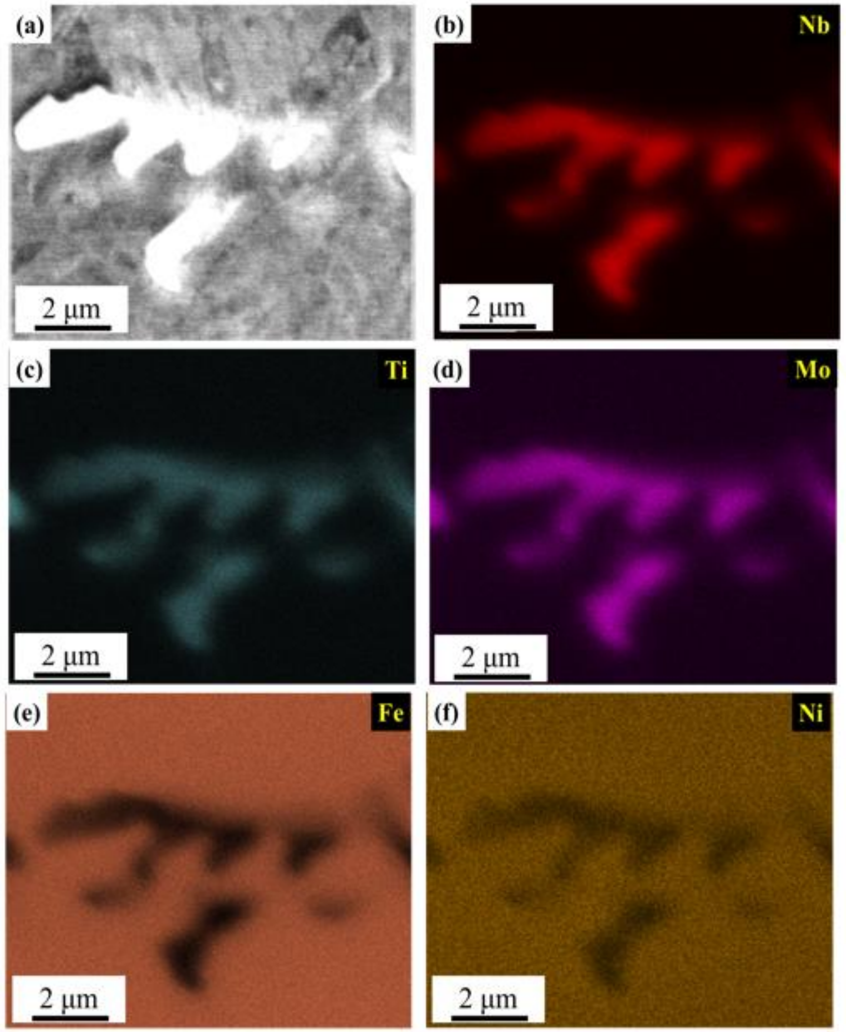


IPF and Phase maps from EBSD across the interface between gradient and 740H

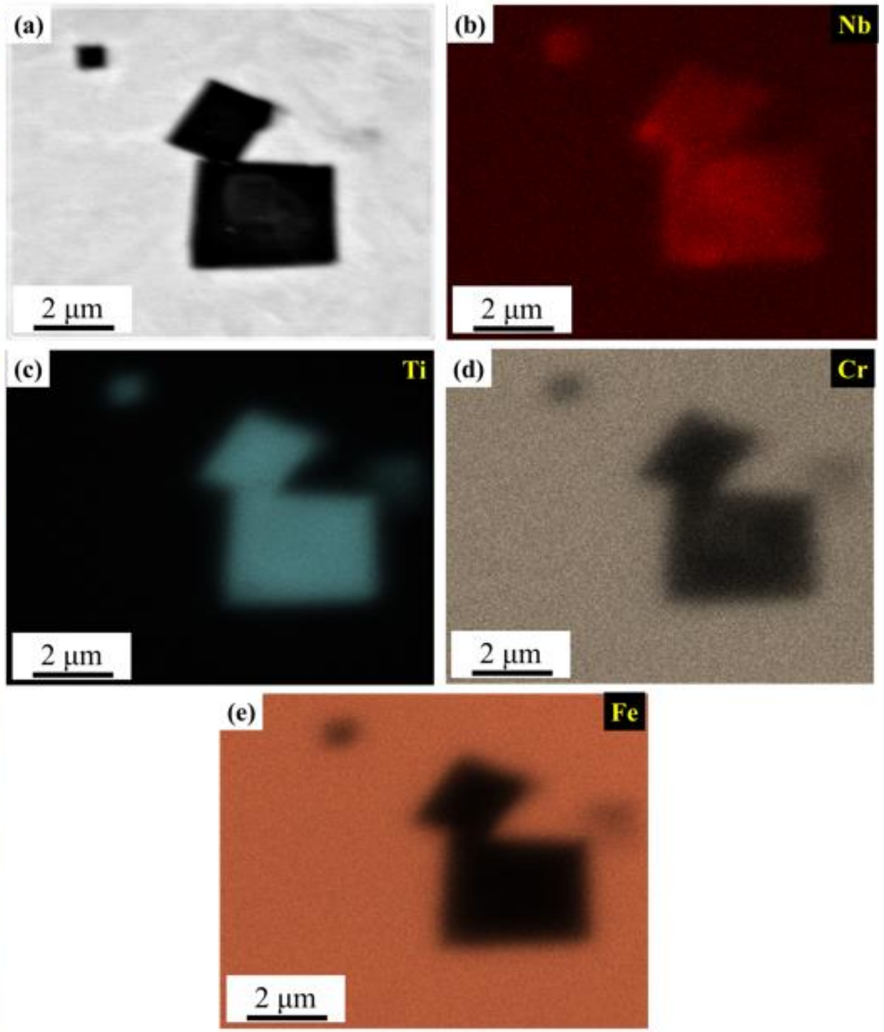
Gradient build with 85% P91 interface



Hardness map



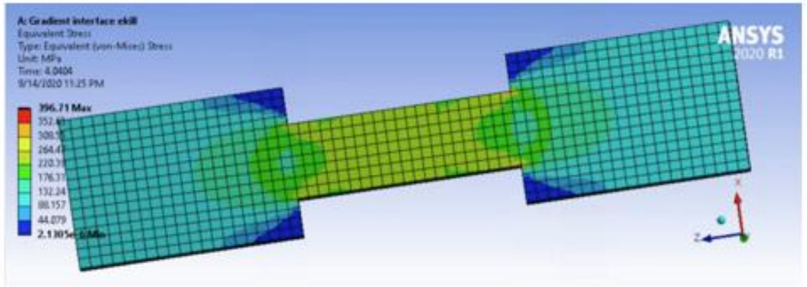
EDS area scan showing the presence of Laves phase rich in Nb, Mo and Ti in the gradient zone



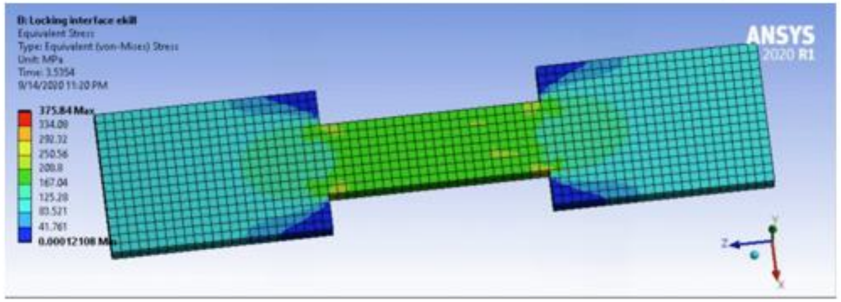
EDS area scan showing the presence of MC carbide rich in Ti and Nb in the gradient zone

Damage comparison using FEM simulations

Joint property: same material property as P91 but with reduced ultimate tensile strength

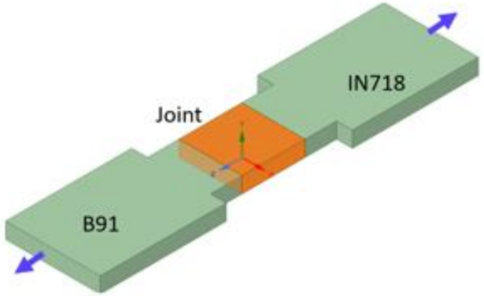


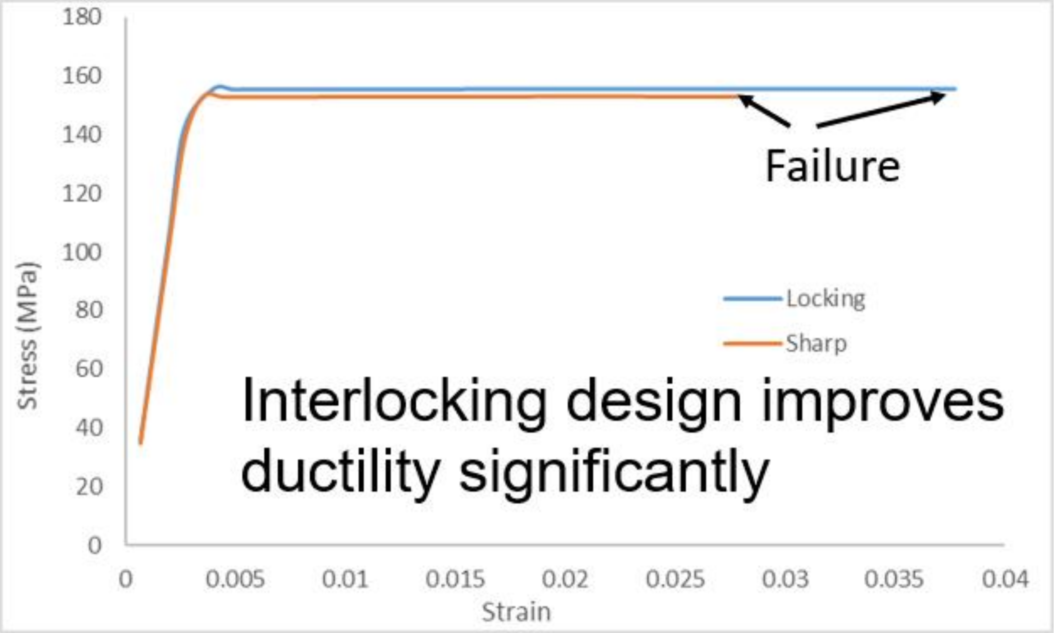
von Mises stress

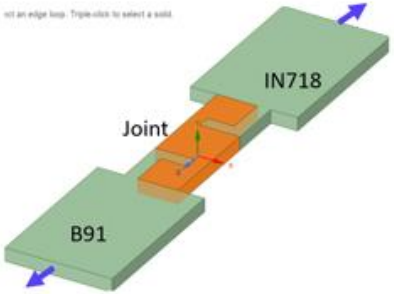


Sharp interface

Interlocking interface







Concluding remarks

Achievements

- Promising results obtained for graded alloy build using WAAM
- A set of ICME tools have been developed and integrated for the design modeling for WAAM of steel, superalloy and their mixture.
- The developed WAAM and heat treatment of P91 and 740H can be further applied to larger components after UQ analysis.

Ongoing research

- Finish analysis and design on the graded alloy by WAAM with post-heat treatment.
- Analysis and design on the intermediate blocks including both WAAM and post-heat treatment.

Plan for improvement

- Further design macro/microstructure interface for improved properties

Journal publications

- Kun Li, Michael A Klecka, Shuying Chen, Wei Xiong*, “Wire-arc additive manufacturing and post-heat treatment optimization on microstructure and mechanical properties of Grade 91 steel”, Additive Manufacturing, Under revision, (2020)

- Santanu Paul, Jian Liu, Seth T. Strayer, Yunhao Zhao, Soumya Sridar, Michael A. Klecka, Wei Xiong, Albert C. To*, "A Discrete Dendrite Dynamics Model for Epitaxial Columnar Grain Growth in Metal Additive Manufacturing with Application to Inconel", Additive Manufacturing, 36 (2020) 101611. https://doi.org/10.1016/j.addma.2020.101611

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