NETL Virtual Project Review Meeting, High Performance Materials, 6/8/2021

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

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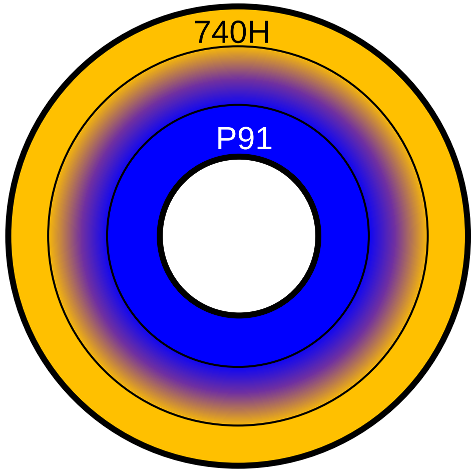
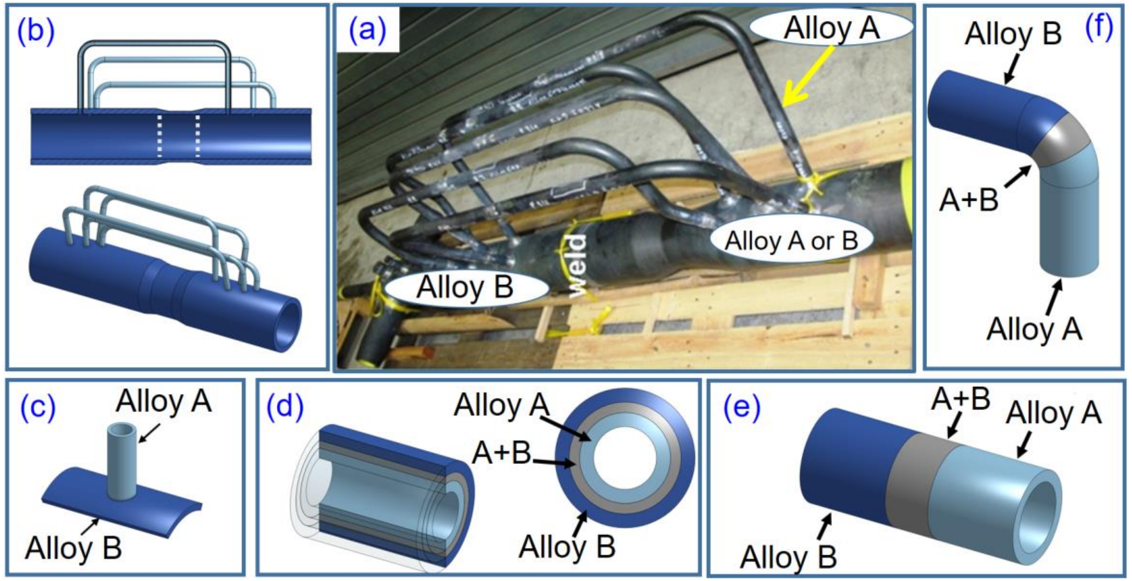
Acknowledgement:

DE-FE0031637

Background and significance

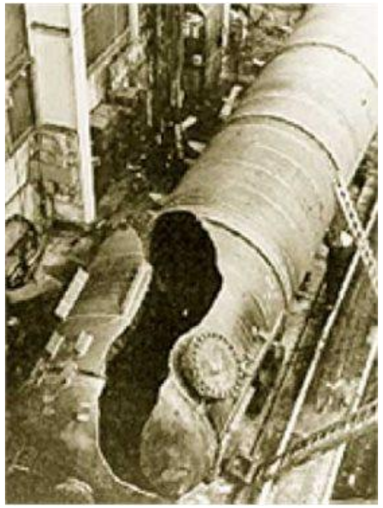
Complex shape manufacturing





Balance between performance and cost

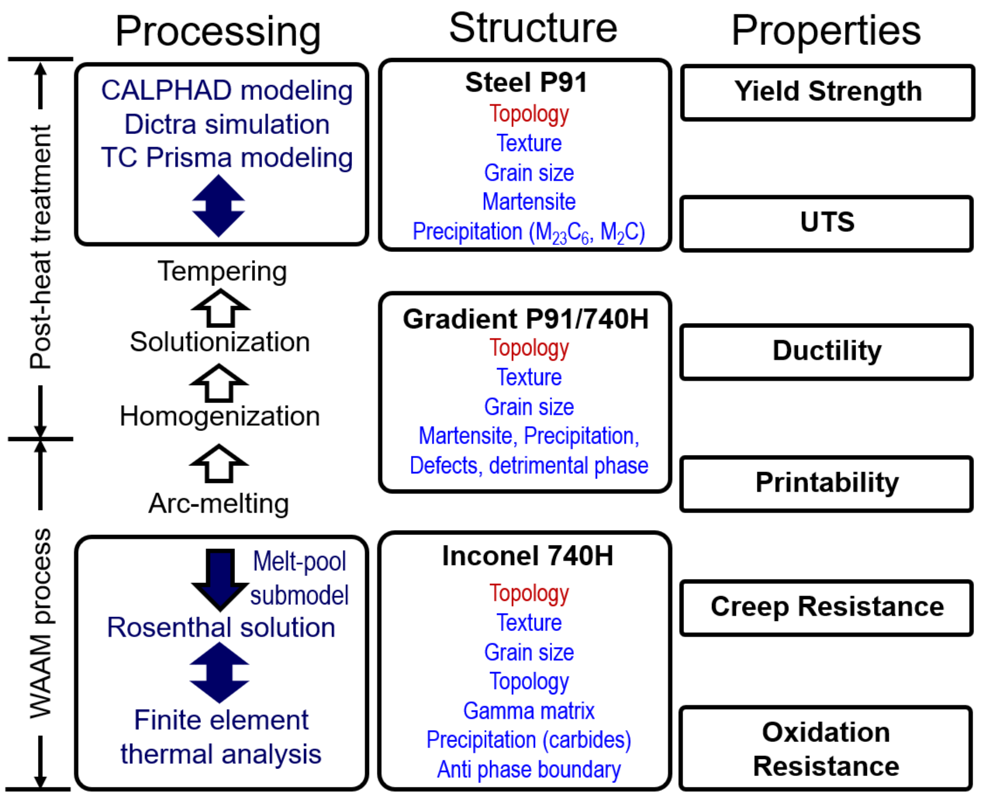
Repair pipeline in a rapid mode



Images from internet

Project objectives

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



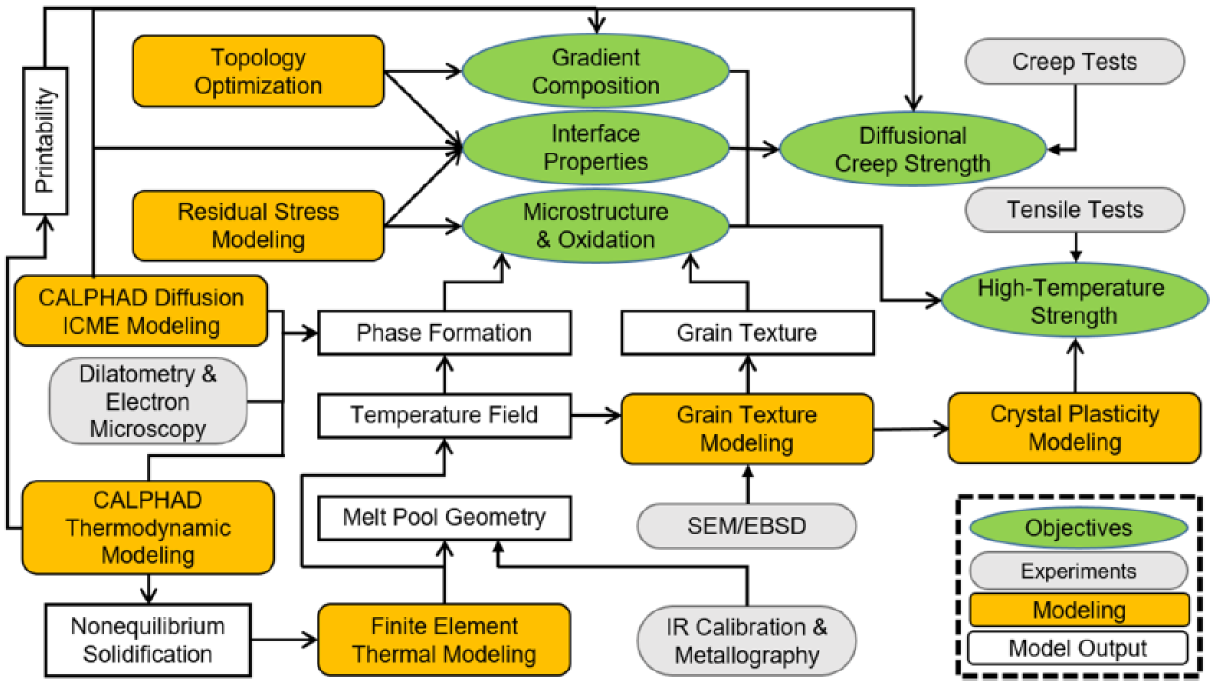
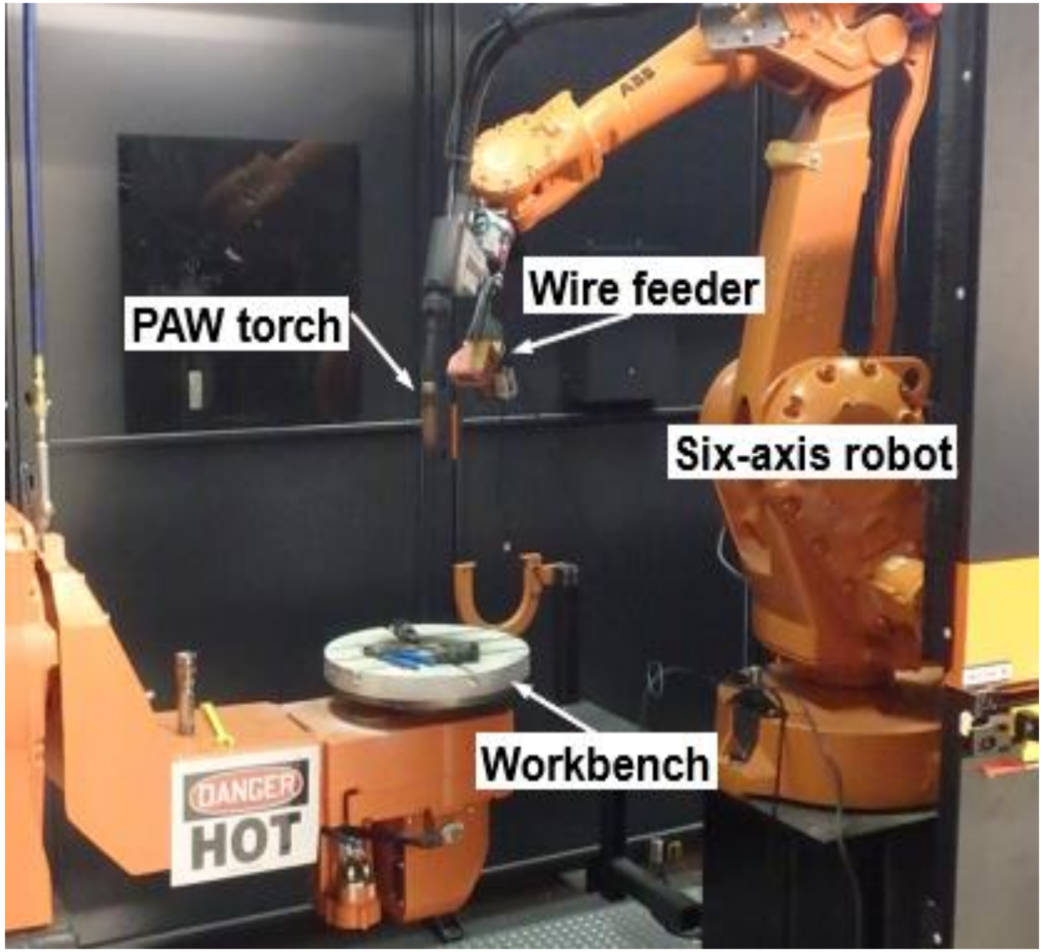


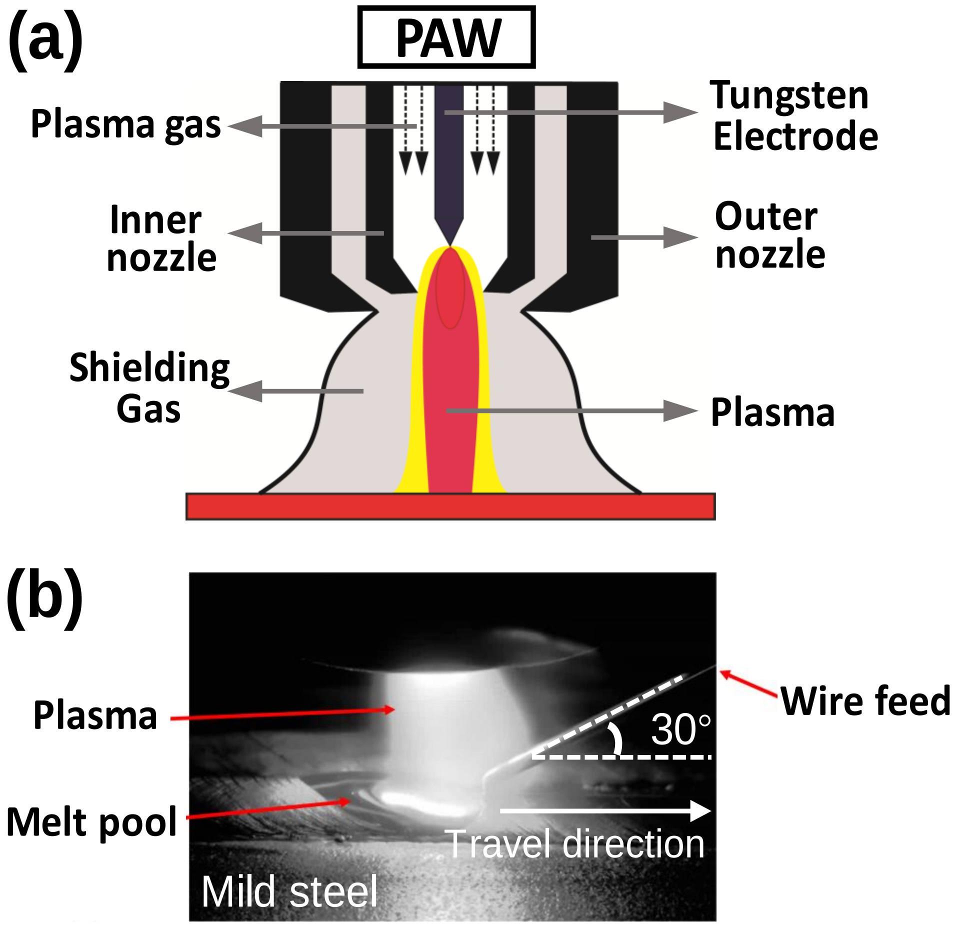
Figure 1. ICME model framework for additive manufacturing of alloys with graded structure.

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

WAAM setup at RTRC

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

(1) Single print and (2) sharp interface print

Design Roadmap

⑥ **3rd generation** printing and testing

⑤a Data driven ML and GA design for intermediate block **(2nd generation)**

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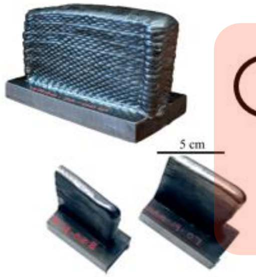
⑤b Interface structure design **(2nd generation)**

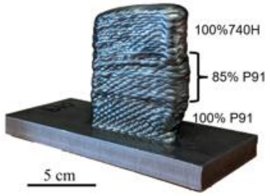
④ Post-heat treatment design on graded alloy builds **(1st generation)**

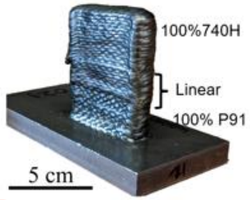
③ Computational design on intermediate blocks

① Inconel 740H & P91 printing and post-heat treatment

② Sharp interface builds for deposition sequence and post-heat treatment

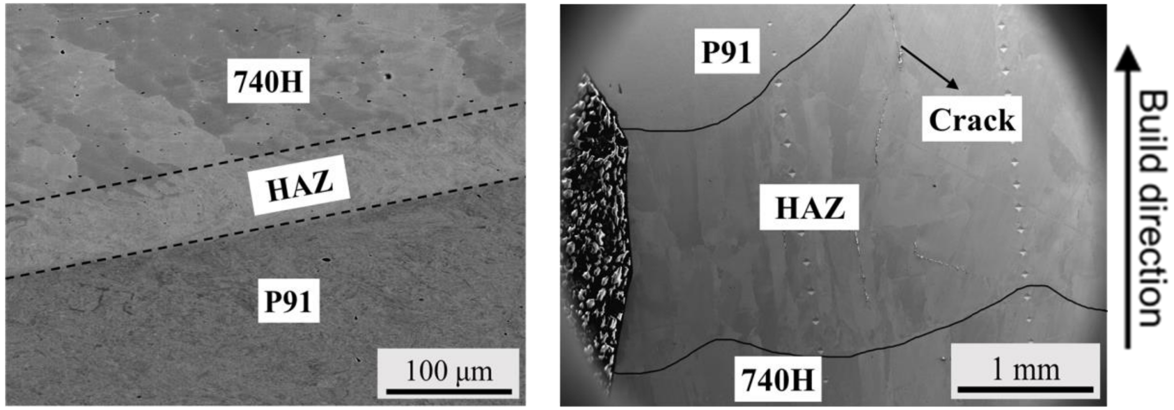






Sharp interface print (740H on P91 vs. P91 on 740H)

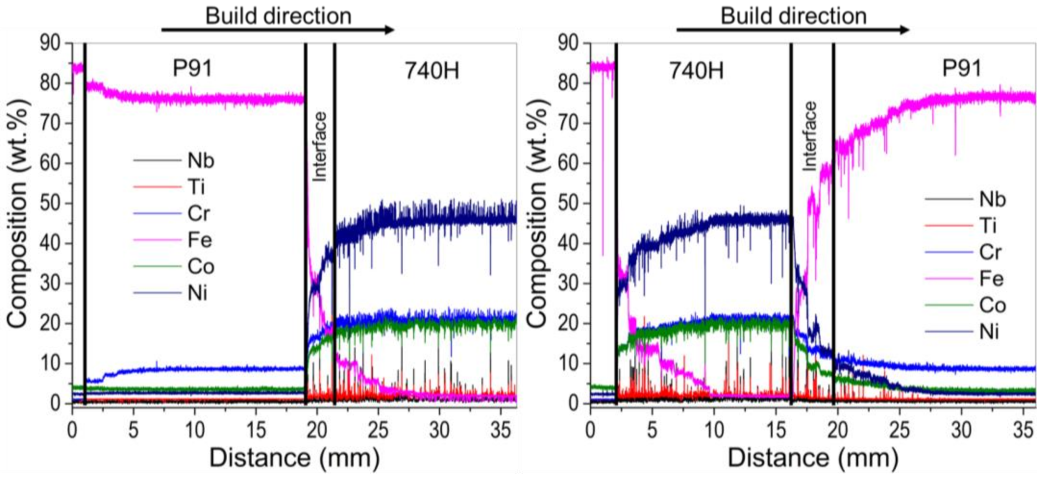
740H on P91 | P91 on 740H



Width of the HAZ ≈ 60 µm | Width of the HAZ ≈ 2200 µm

SEM micrographs across the gradient zone showing a wider HAZ with cracks in P91 over 740H deposit

740H on P91 | P91 on 740H

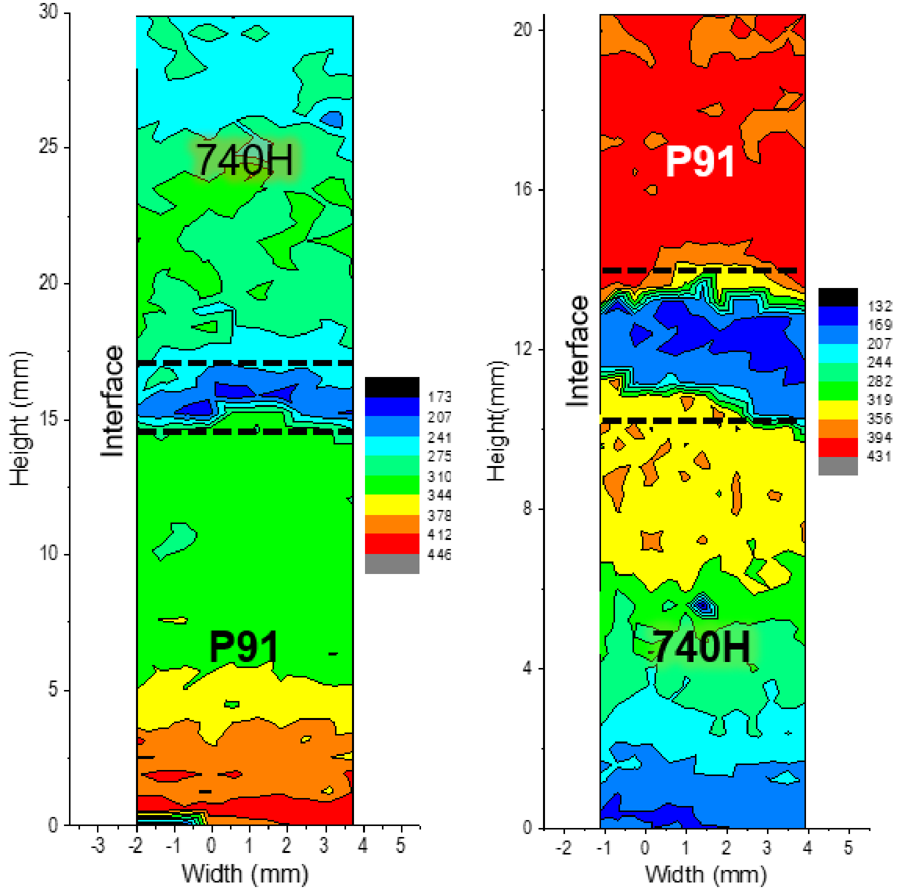


EDS composition profile along the build direction showing higher dissolution of Fe in 740H observed in 740H over P91 build

Lower hardness at interface between P91 and 740H

Lower hardness at interface between P91 and 740H as well as 740H and substrate

740H on P91 | P91 on 740H



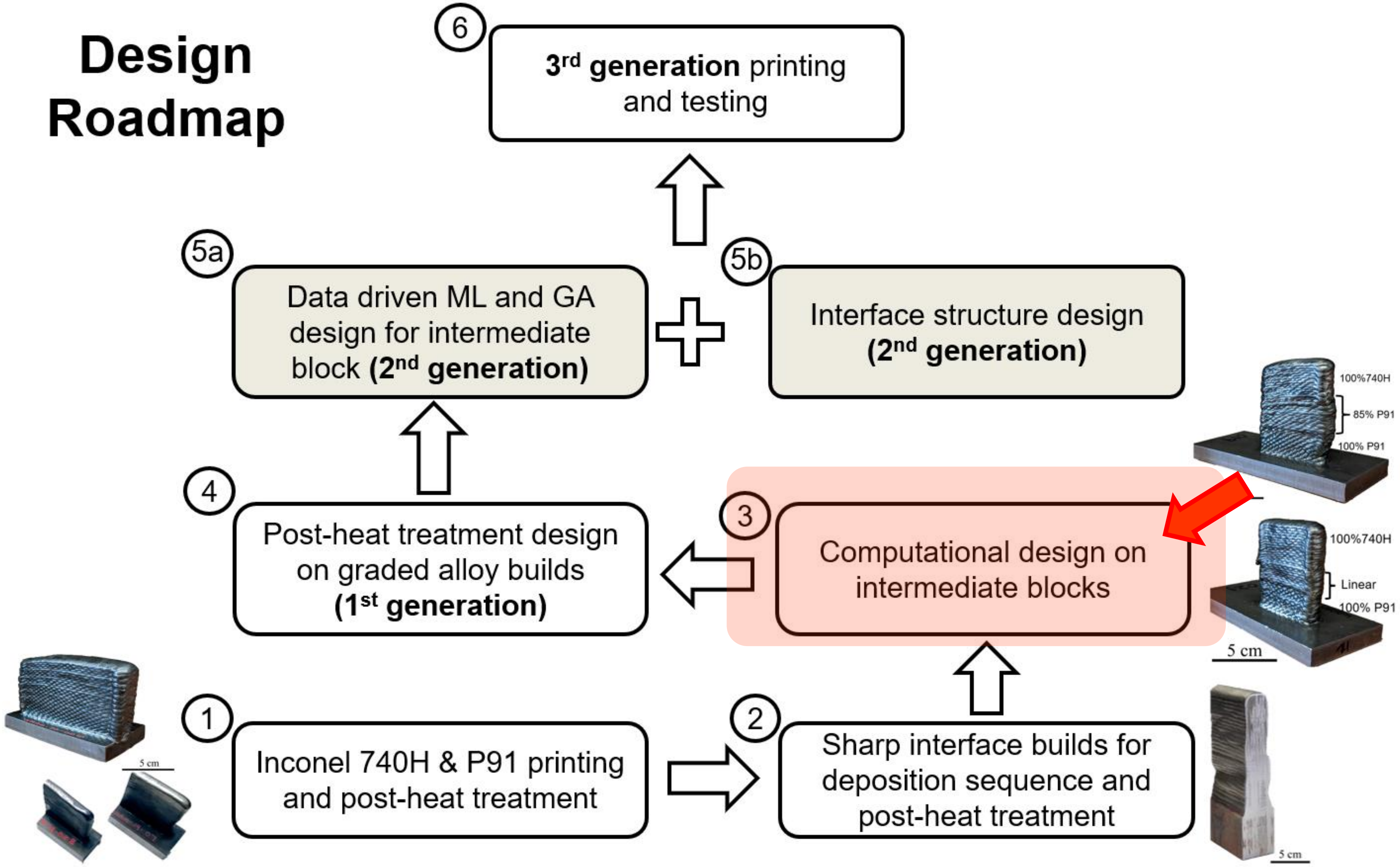
Hardness maps along the build direction

Sharp interface print

740H over P91 is the optimum deposition sequence for P91/740H bimetallic structures

740H on P91	P91 on 740H
No detrimental phases or cracks at interface	Cracks observed at the interface
Smaller gradient zone	Wider gradient zone
Fine grains at interface	Coarse grains at interface
Higher dissolution of Fe into 740H for longer distance away from the interface	Lesser diffusion of Ni into P91 away from the interface
Lower hardness at interface between P91 and 740H	Lower hardness at 1) interface between P91 and 740H 2) interface between 740H and mild steel substrate

(3) Computational design of the Gen 1 graded alloy builds



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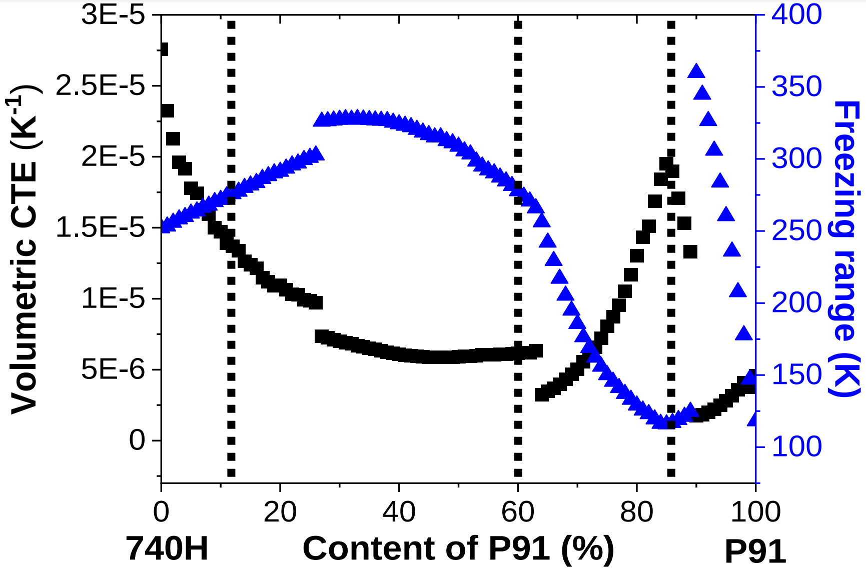
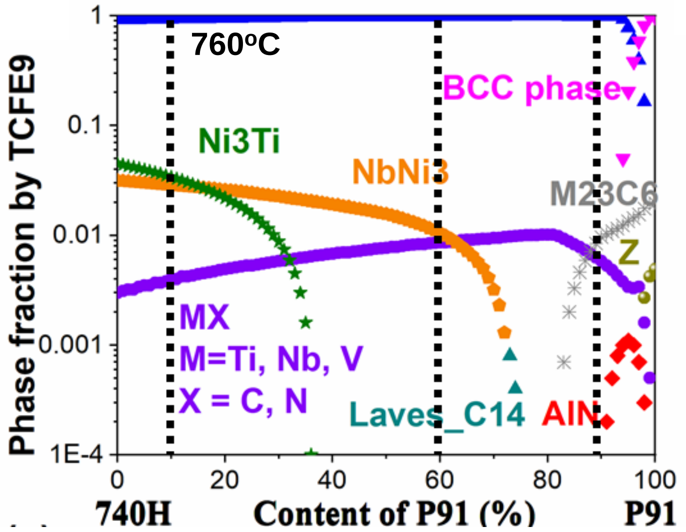
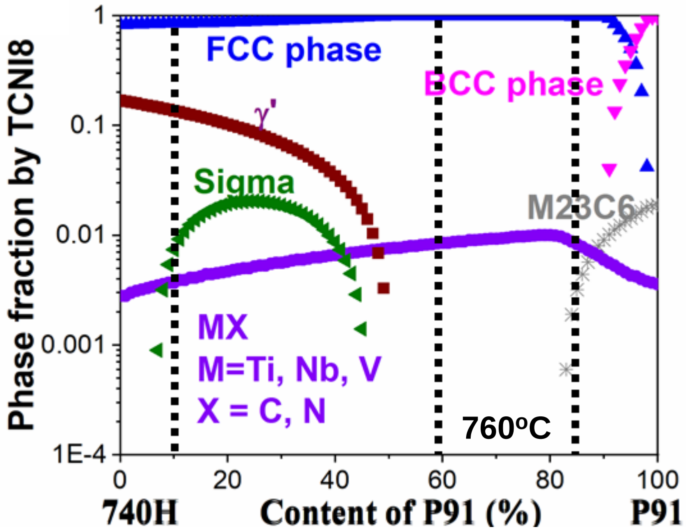
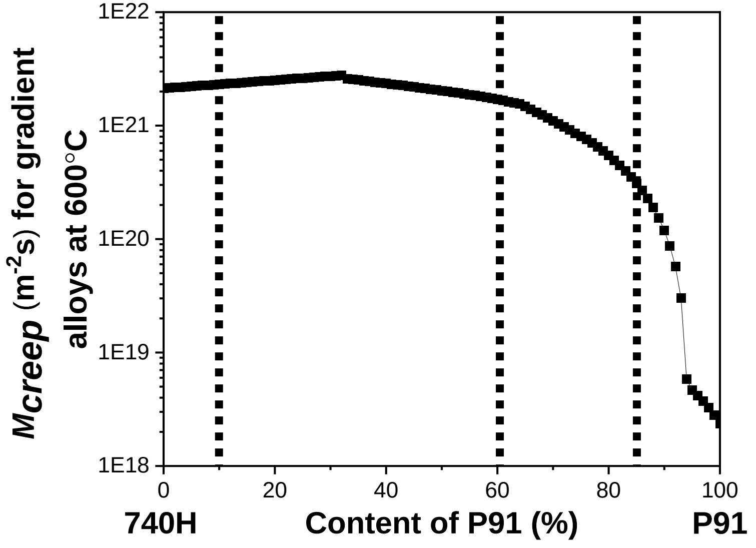
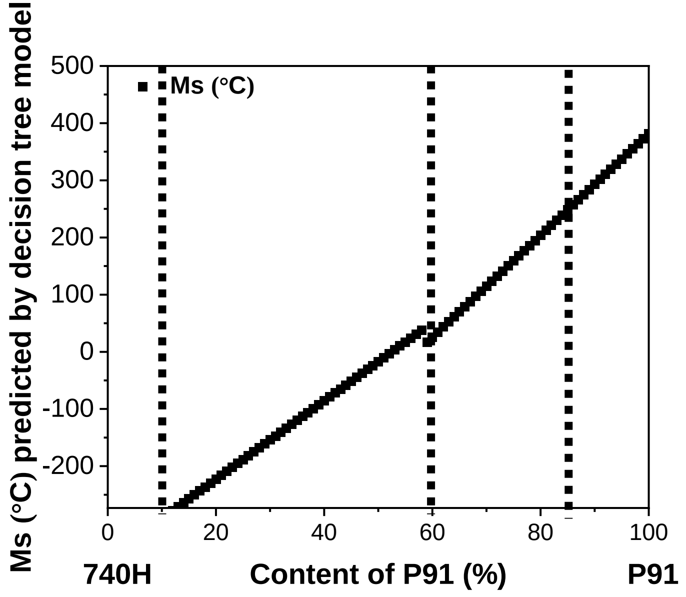
Computational design of the Gen 1 graded alloy builds





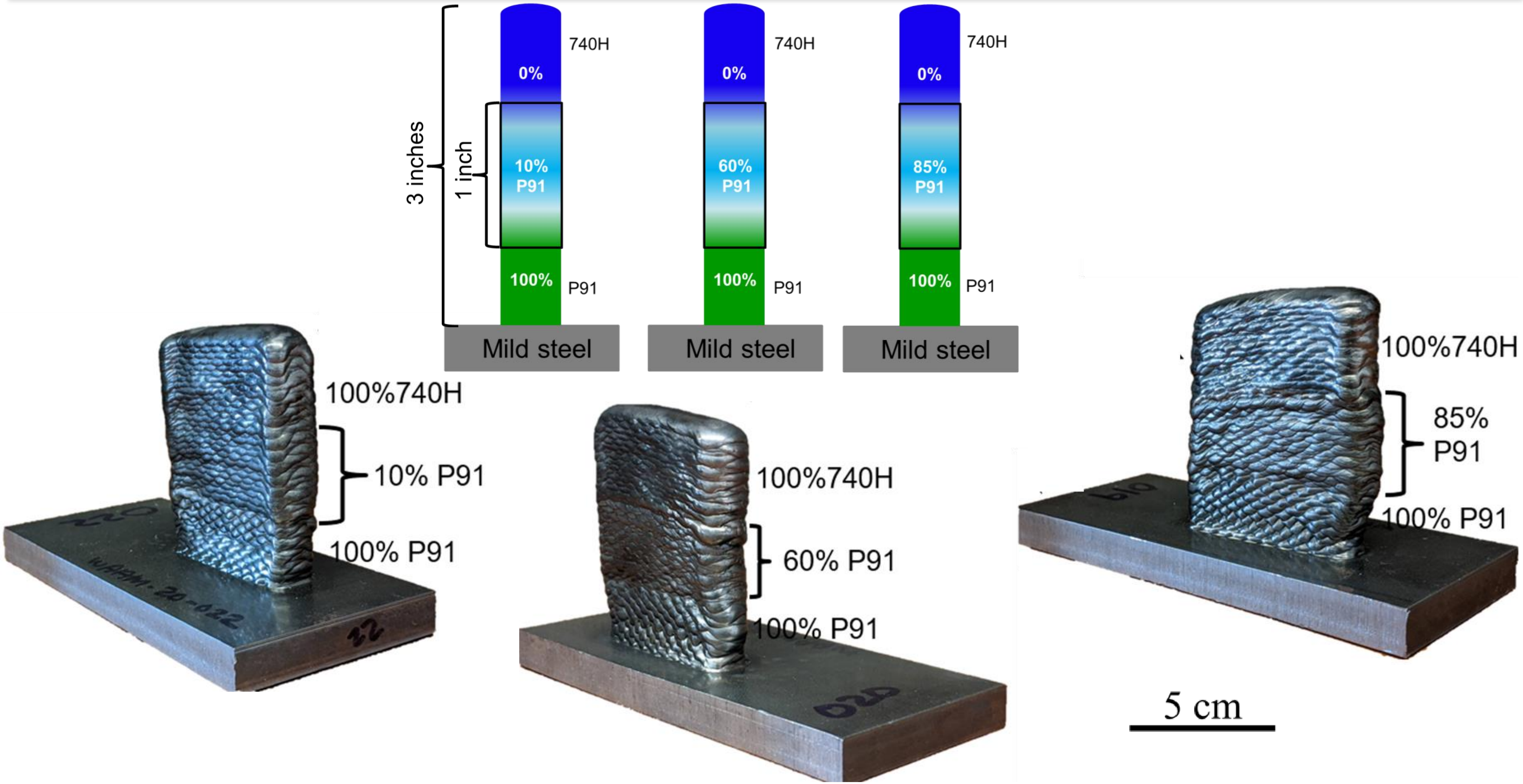






Compositions chosen:
1) 10 wt.% P91
2) 60 wt.% P91
3) 85 wt.% P91

Gen 1 graded alloy builds with interface: 10%, 60%, and 85% P91

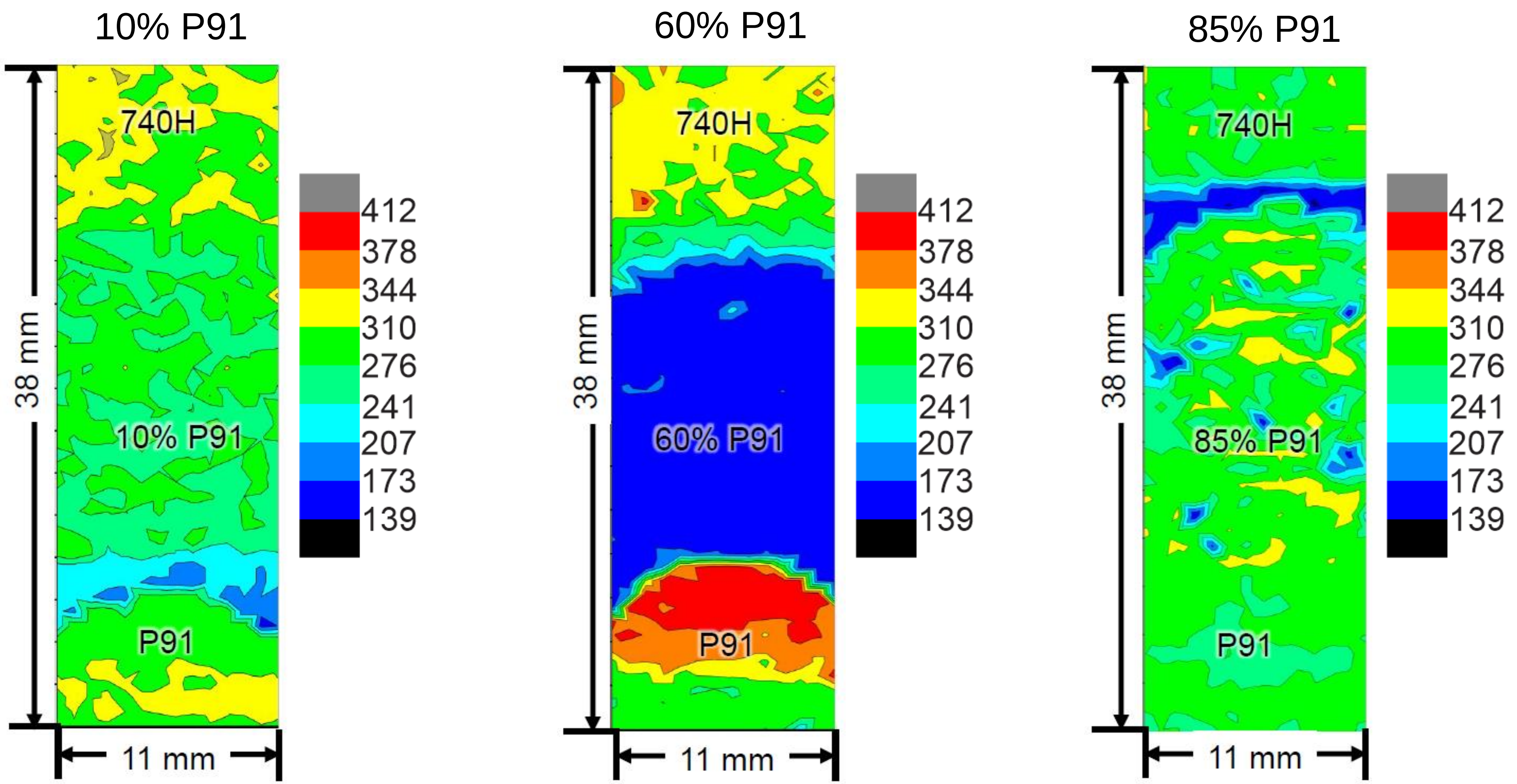


As-built alloys with interface: 10%, 60%, and 85% P91 (Hardness Map)

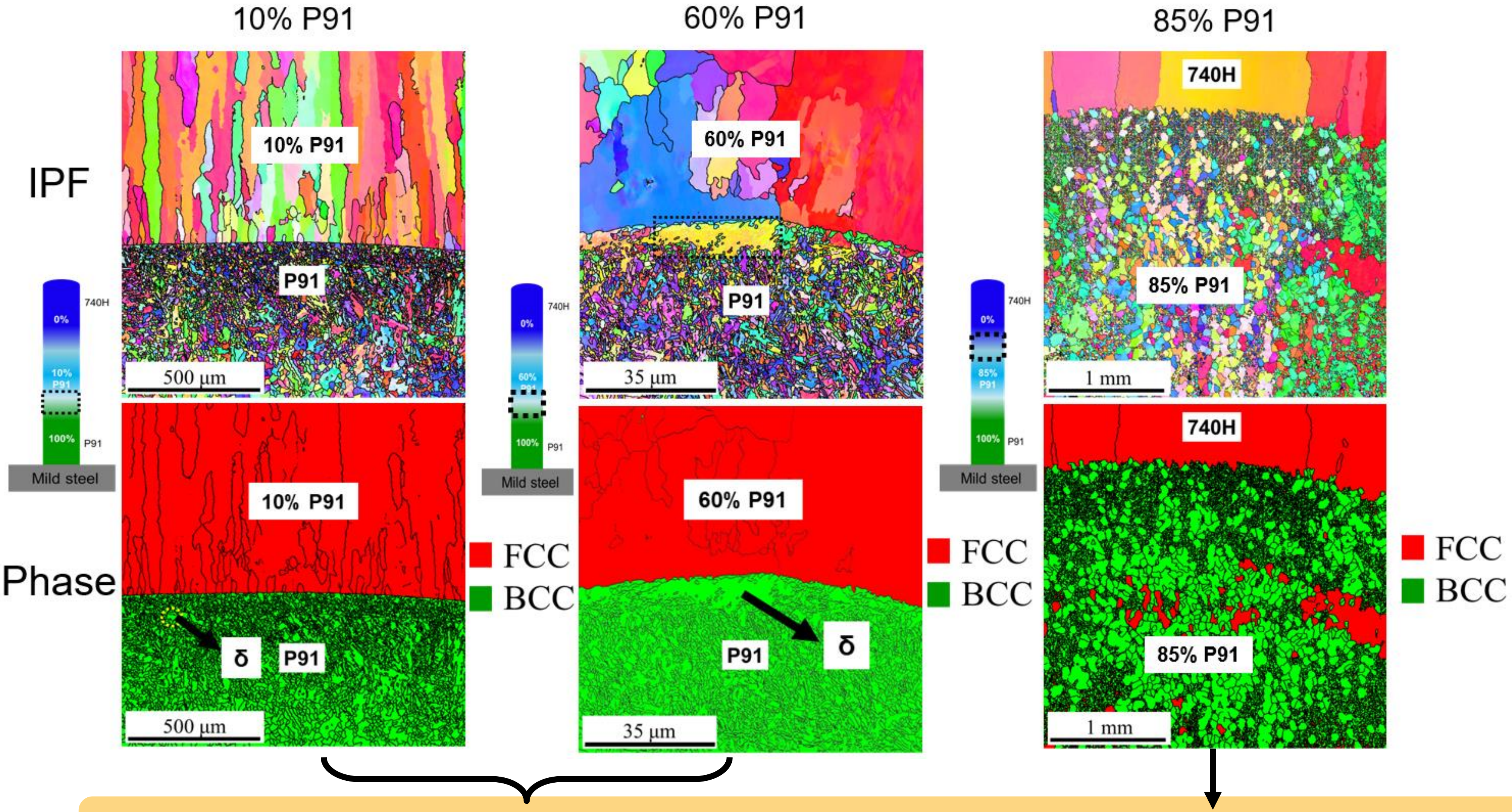
predominantly uniform hardness

Gradient interface has lowest hardness

predominantly uniform hardness



As-built alloys with interface: 10%, 60%, and 85% P91 (Microstructure)



- Gradient interface has an FCC structure.
- The presence of δ-ferrite is in the P91 close to the interface

- Gradient interface has a BCC structure mainly.
- No δ-ferrite exists close to the interface

(4) Post-heat treatment of graded alloy builds

Design Roadmap

6 — **3rd generation** printing and testing

5a — Data driven ML and GA design for intermediate block **(2nd generation)**

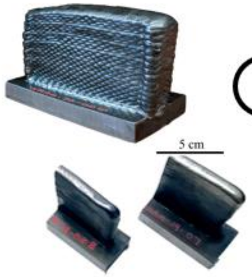
5b — Interface structure design **(2nd generation)**

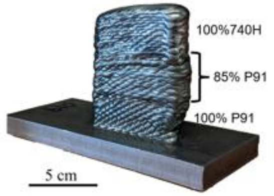
4 — Post-heat treatment design on graded alloy builds **(1st generation)**

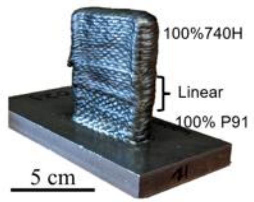
3 — Computational design on intermediate blocks

2 — Sharp interface builds for deposition sequence and post-heat treatment

1 — Inconel 740H & P91 printing and post-heat treatment

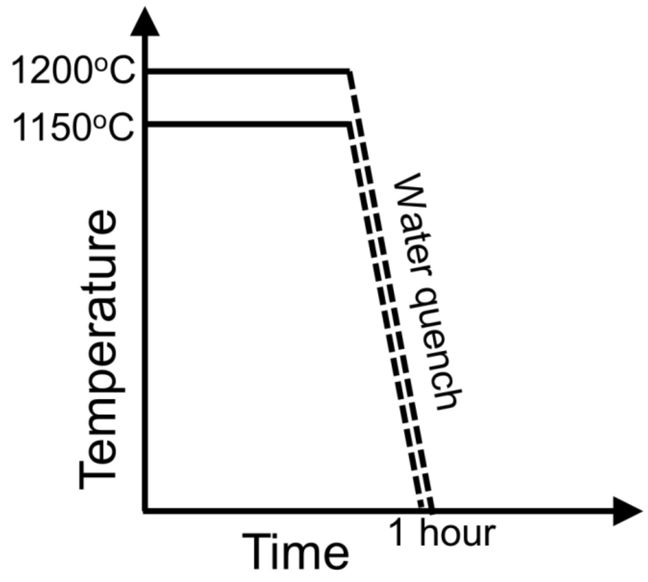






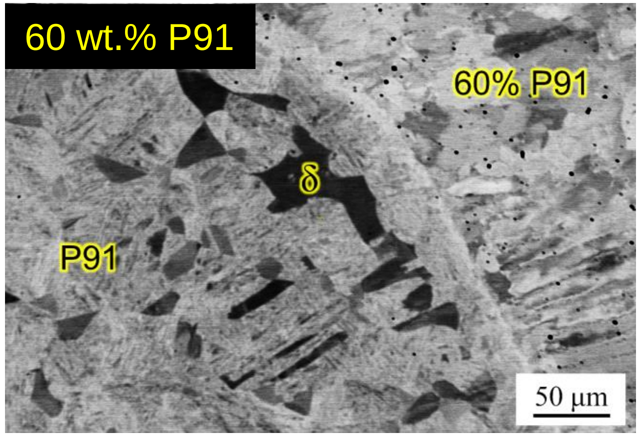
Homogenization studies for Gen 1 graded alloys (**1200ºC**/1 hour)

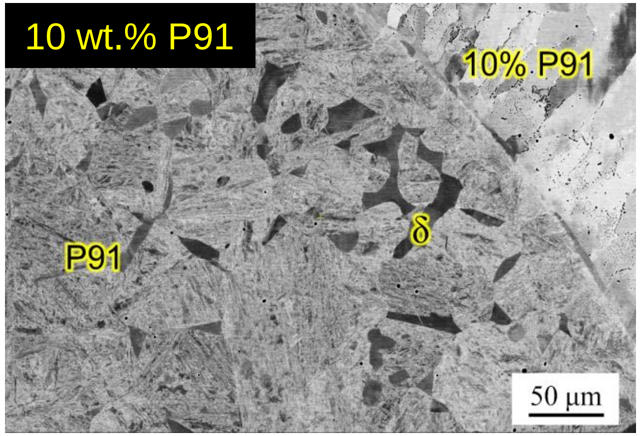
Homogenization at 1200ºC for 1 hour was chosen based on the post-heat treatment designed for sharp gradient builds



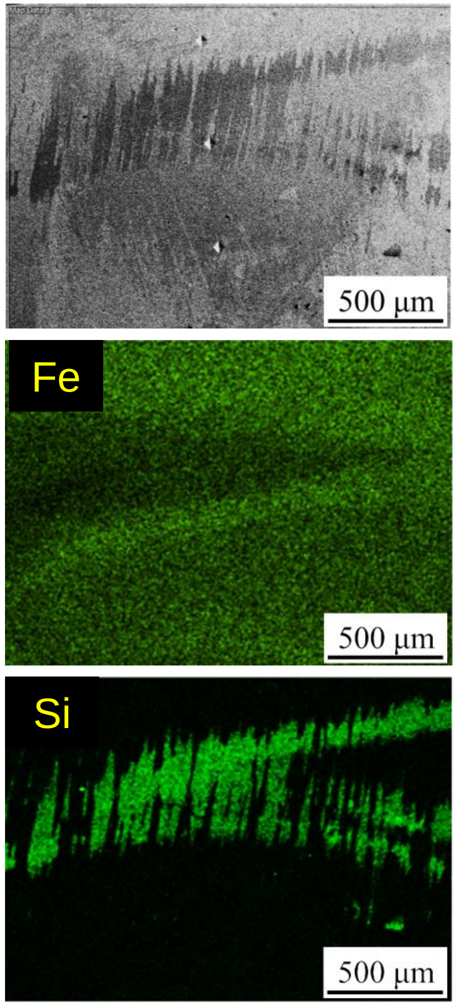
Homogenization at 1200ºC for 1 hour yielded:
- ✓ *Clean interfaces in 85 wt.% P91 graded alloy*
- ✓ *δ-ferrite formation in P91 at P91/gradient interface in 60 wt.% graded alloy*
- ✓ *δ-ferrite formation and Si segregation in P91 at P91/gradient interface in 10 wt.% graded alloy*

Presence of δ-ferrite in the P91 side of P91/gradient interface in 60 and 10 wt.% P91 graded alloys.

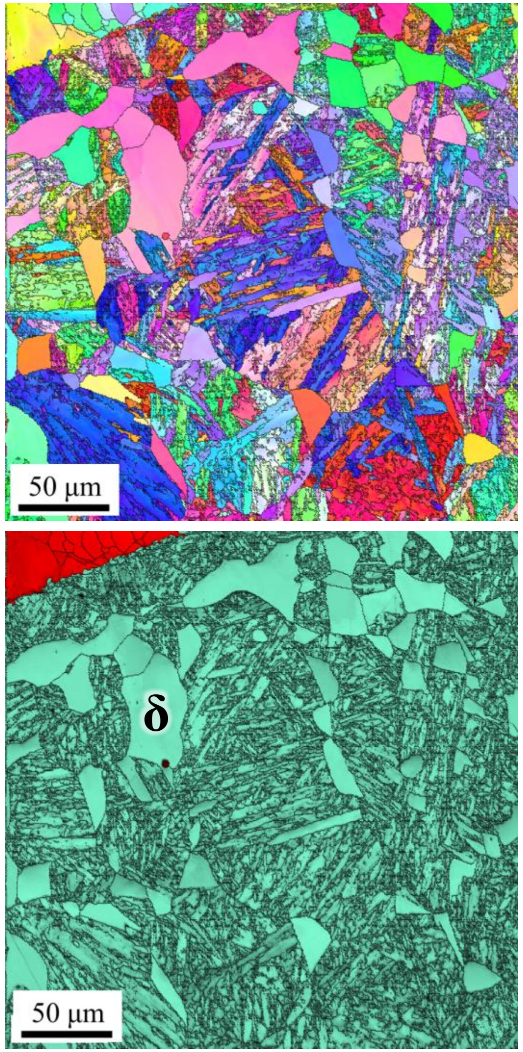




*EDS maps confirming the **segregation of Si** in the P91/gradient interface in 10 wt.% P91 graded alloy*

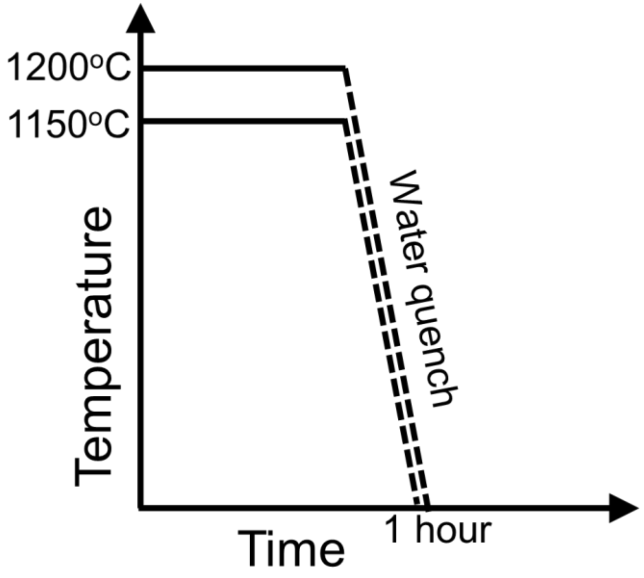


*IPF and IQ+Phase maps confirming the presence of **δ-ferrite in 60 wt.% P91 graded alloy***

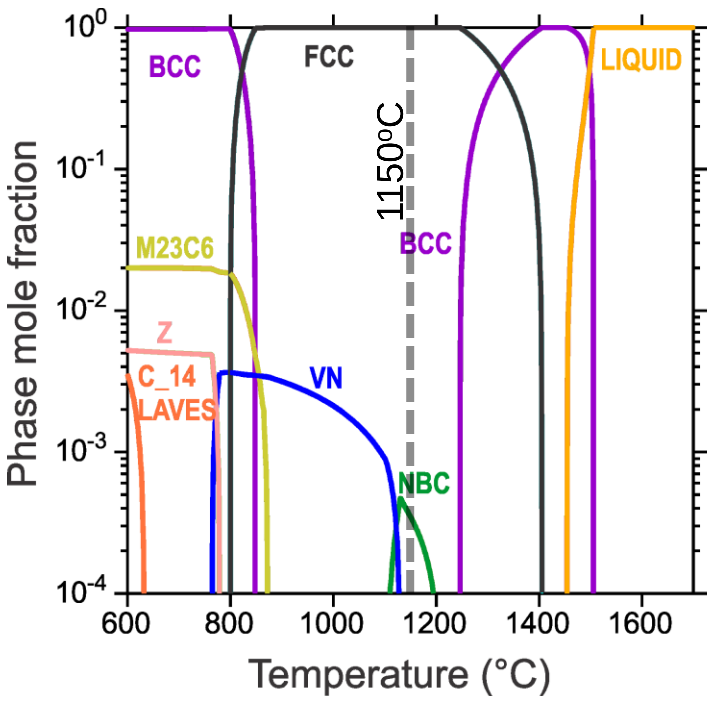


Homogenization studies for Gen 1 graded alloys (**1150ºC**/1 hour)

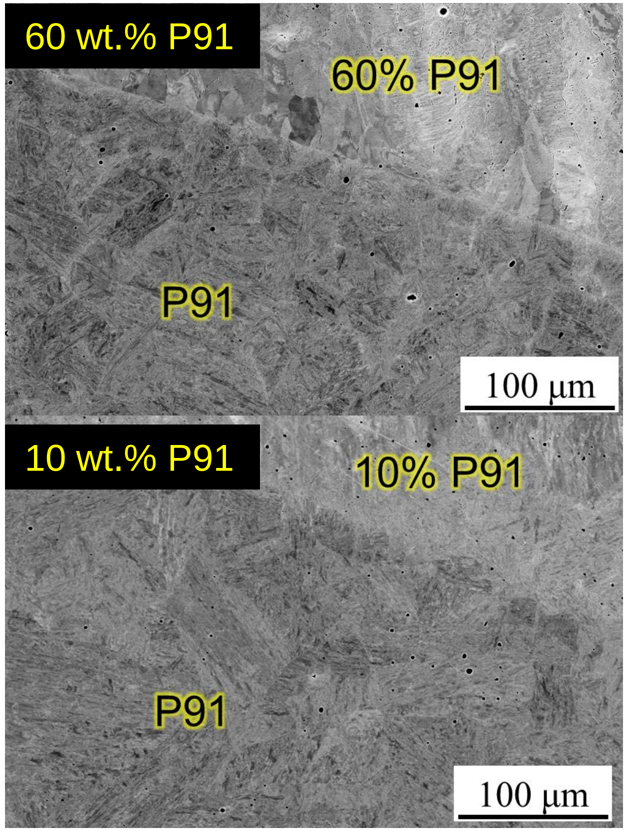
- Homogenization at ***1150ºC for 1 hour*** was found to be the optimum
  - Segregation of Si and δ-ferrite formation was not observed at the interface
- From the calculated equilibrium phase fraction for P91 steel, it was found that 1150ºC is well below the temperature at which δ-ferrite starts to form



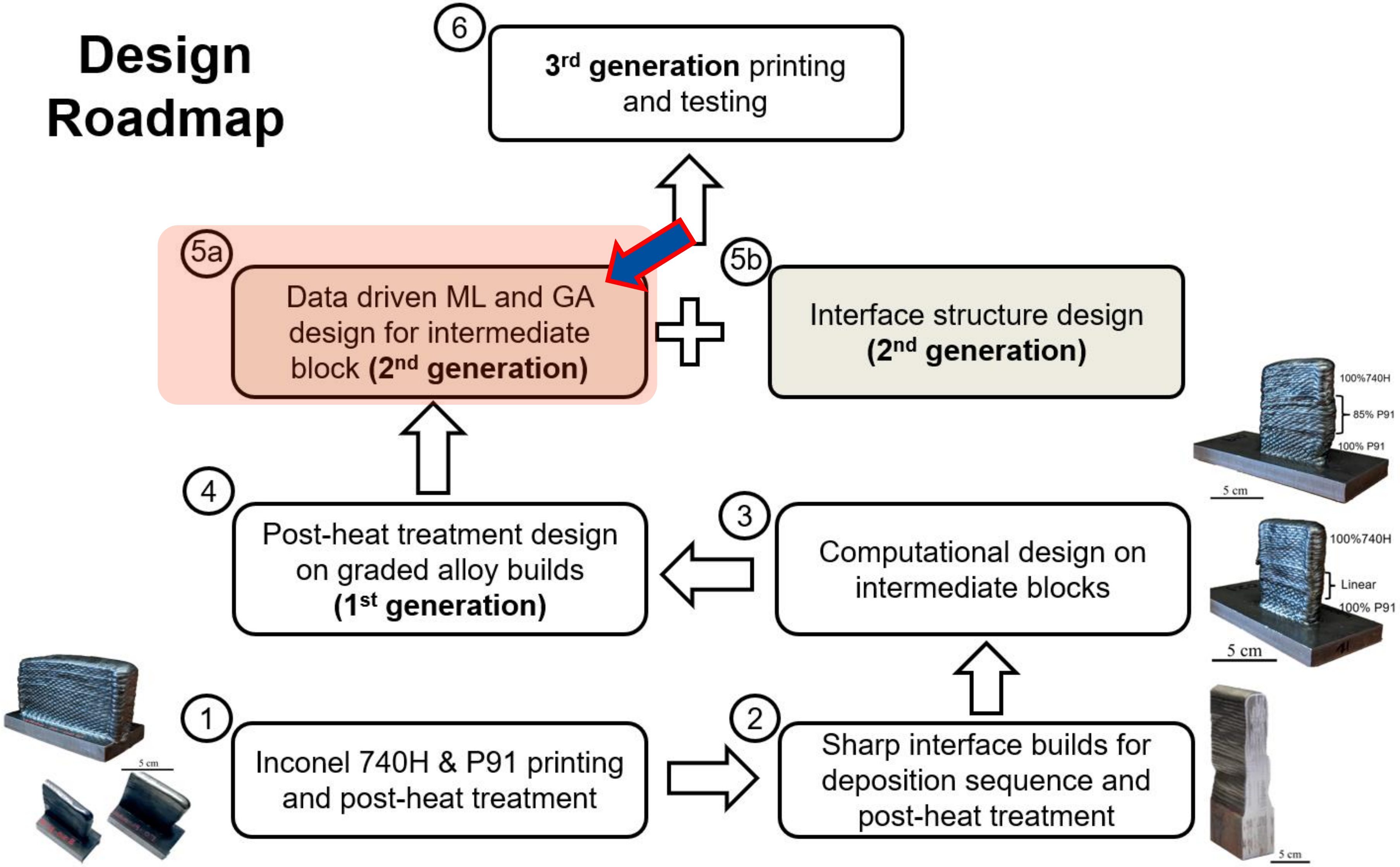
*Clean interfaces without δ-ferrite formation and Si segregation **after homogenization at 1150ºC for 1 hour** in 10 and 60 wt.% P91 graded alloys*



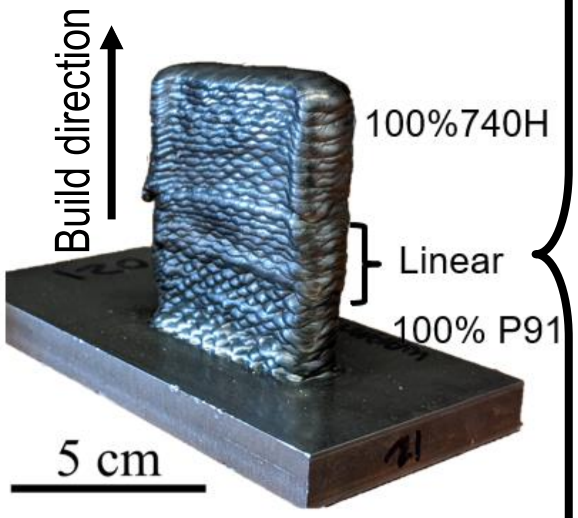
Calculated equilibrium phase fraction as a function of temperature for P91 steel

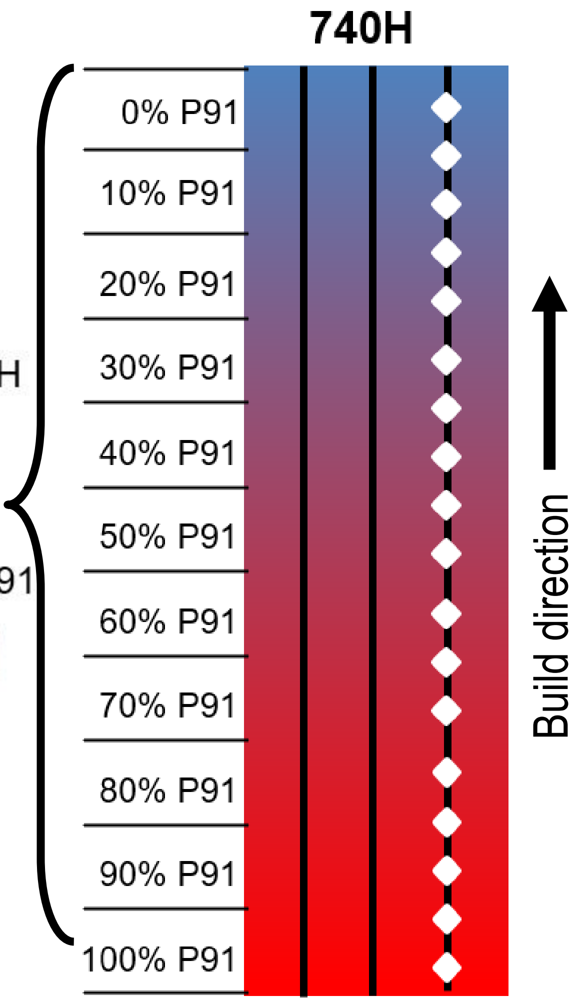


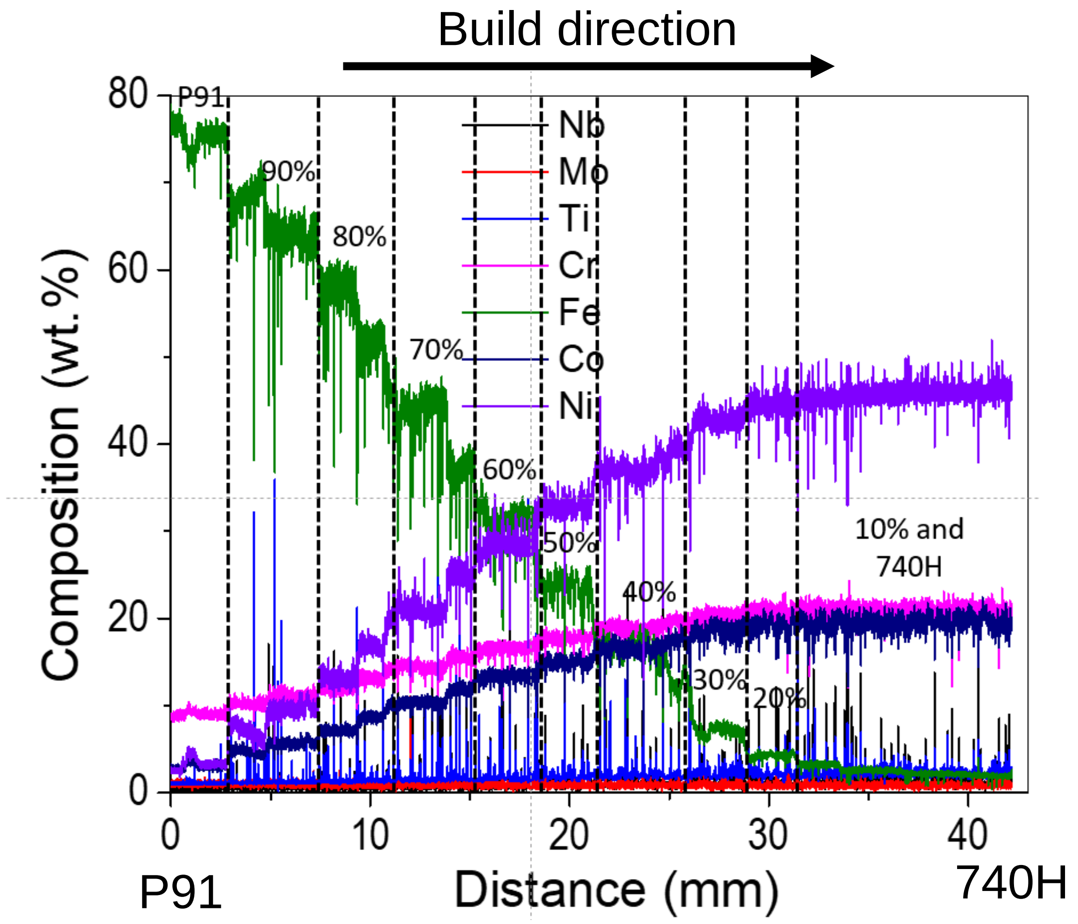
(5a) Data driven ML and GA design for intermediate block (2nd Gen)



Linear build supporting data driven modeling



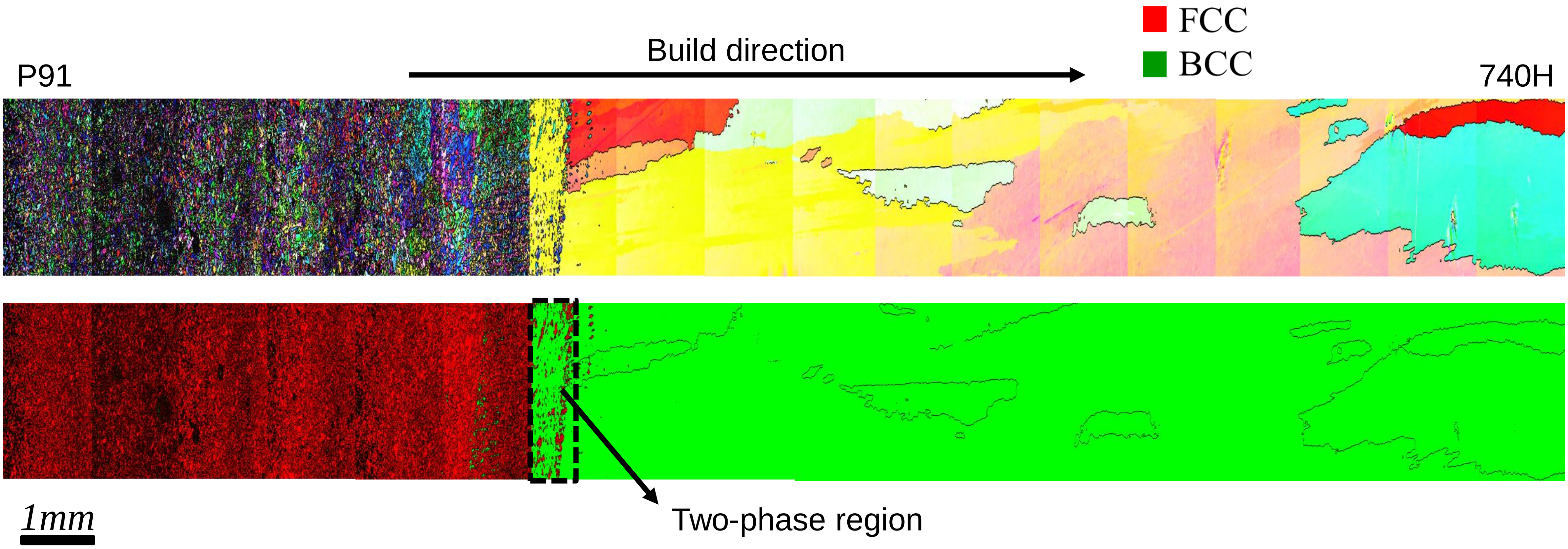




Composition profile along the build direction for the linear gradient alloy

As-built linear graded alloy

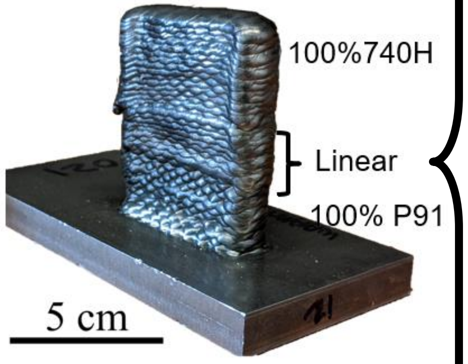
***Inverse pole figure** and **Phase maps** along the build direction*

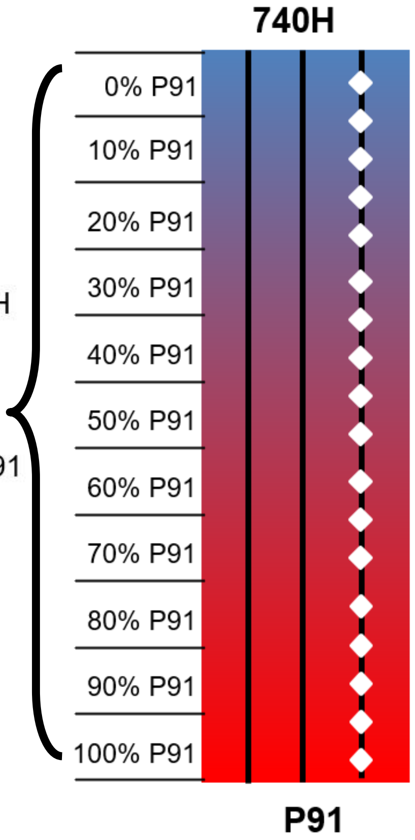


Total length covered ~ 22 mm

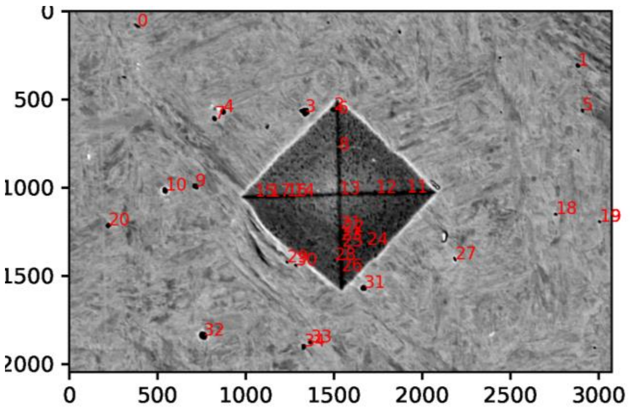
Data driven modeling for composition design

Gradient build via WAAM

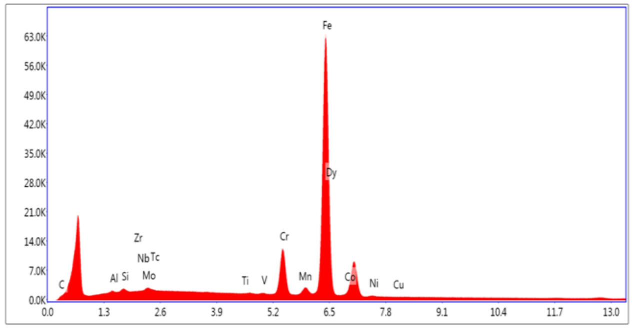




Microstructure and Hardness

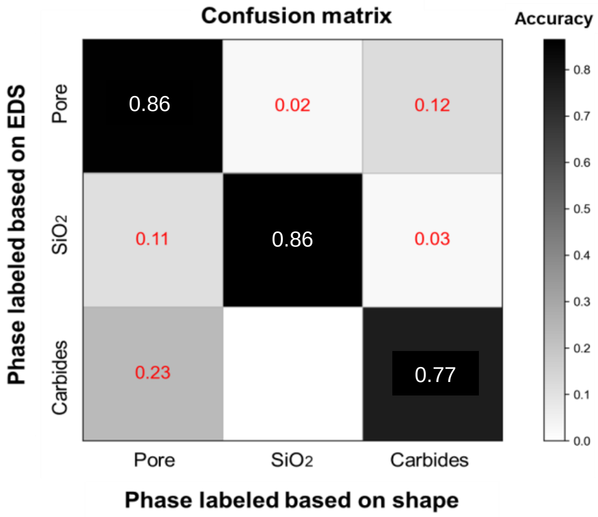


Hardness measurement
3 x 145 indents



EDS measured composition
3 x 145 x 4 point

Pore/Carbides/Phase identification 3 x 145 indents



Data driven modeling for composition design (cont'd)

Measured features:
- Composition
- Matrix phase
- etc.

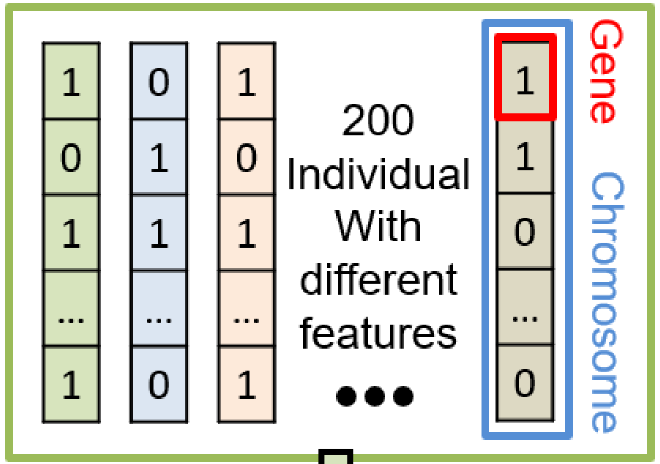
Calculation features:
- Freezing range
- Phase fractions
- Entropy
- etc.

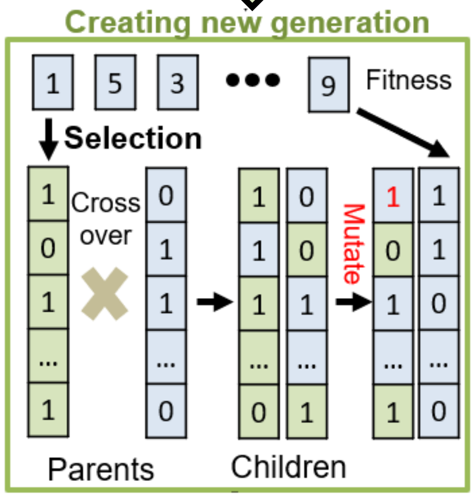
Correlation analysis

SHAP analysis

Measured properties:
- Printability (Porosity)
- Strength (Hardness)
- Ductility (Cracks during hardness test)

SHAP(Shapley Additive exPlanations)

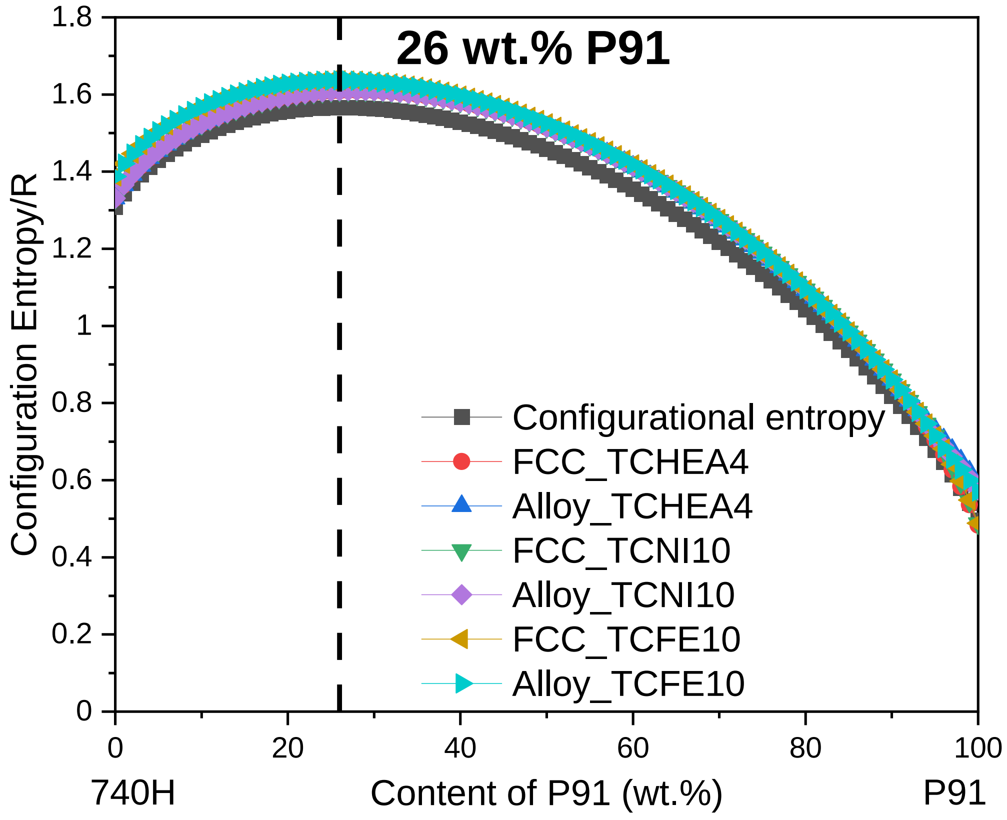




Compositions chosen:
1) 90 wt.% P91 [based on modeling]
2) 26 wt.% P91 [based on entropy]

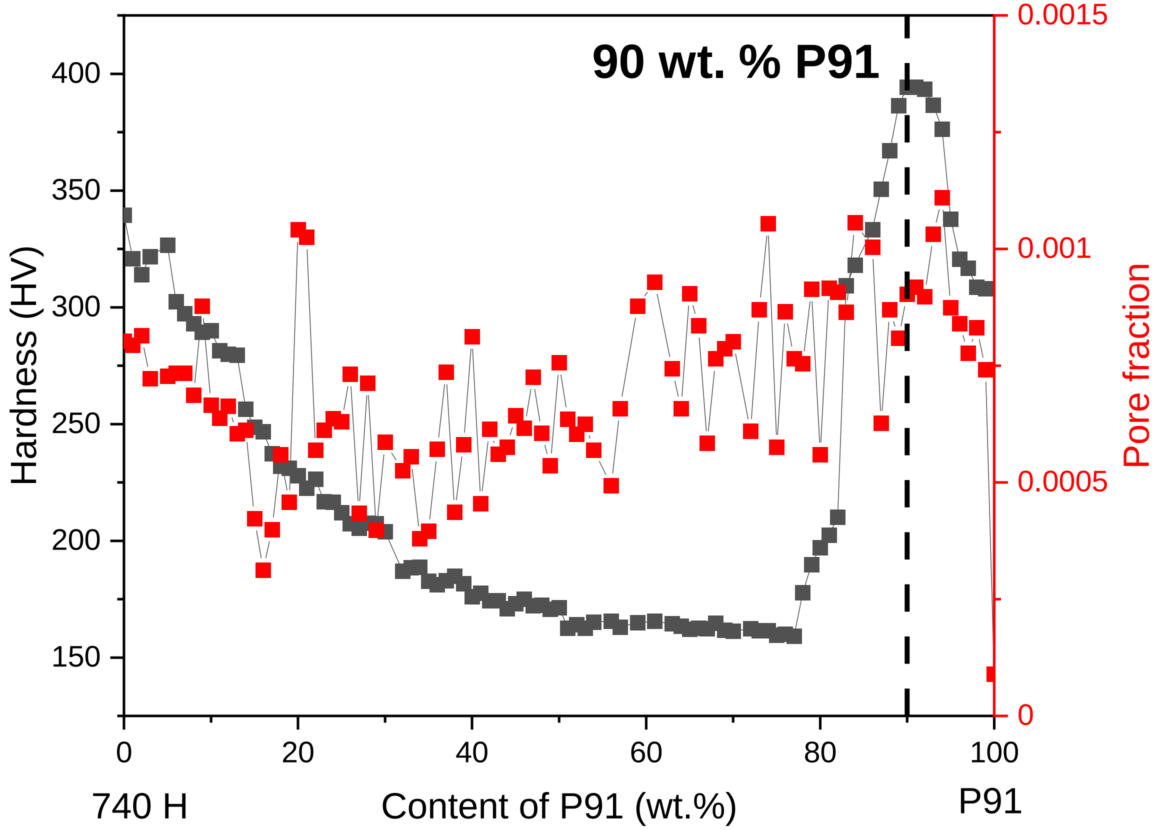
Data driven modeling for composition design (cont'd)

Design results based on High Entropy



Based on CALPHAD model, the 26 wt.% P91 has the highest entropy

Design results based on Machine Learning



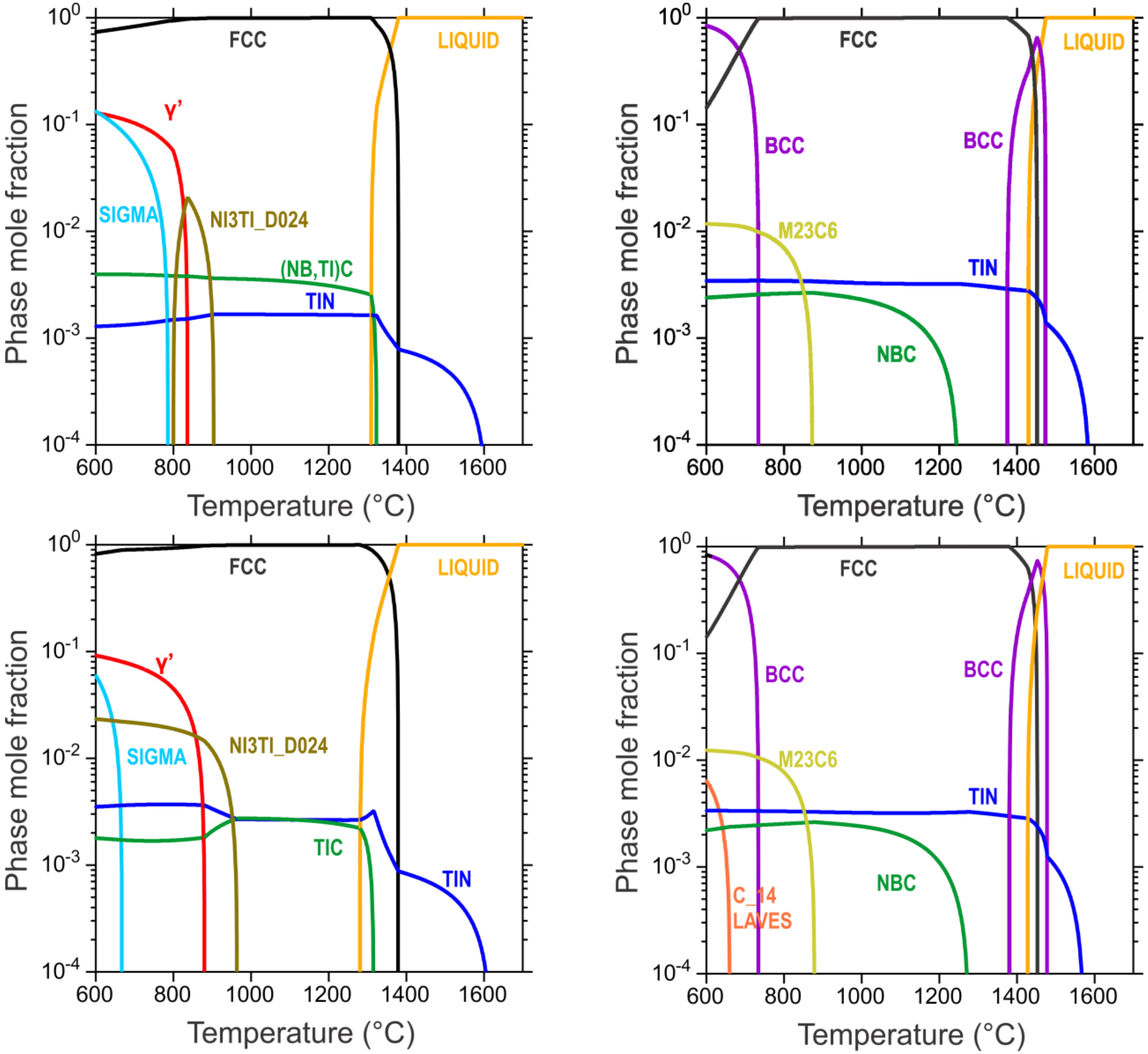
Based on ML models, the 90 wt.% P91 has relatively low porosity and high hardness.

Step and Scheil diagrams for selected compositions

26 wt.% P91 | 90 wt.% P91

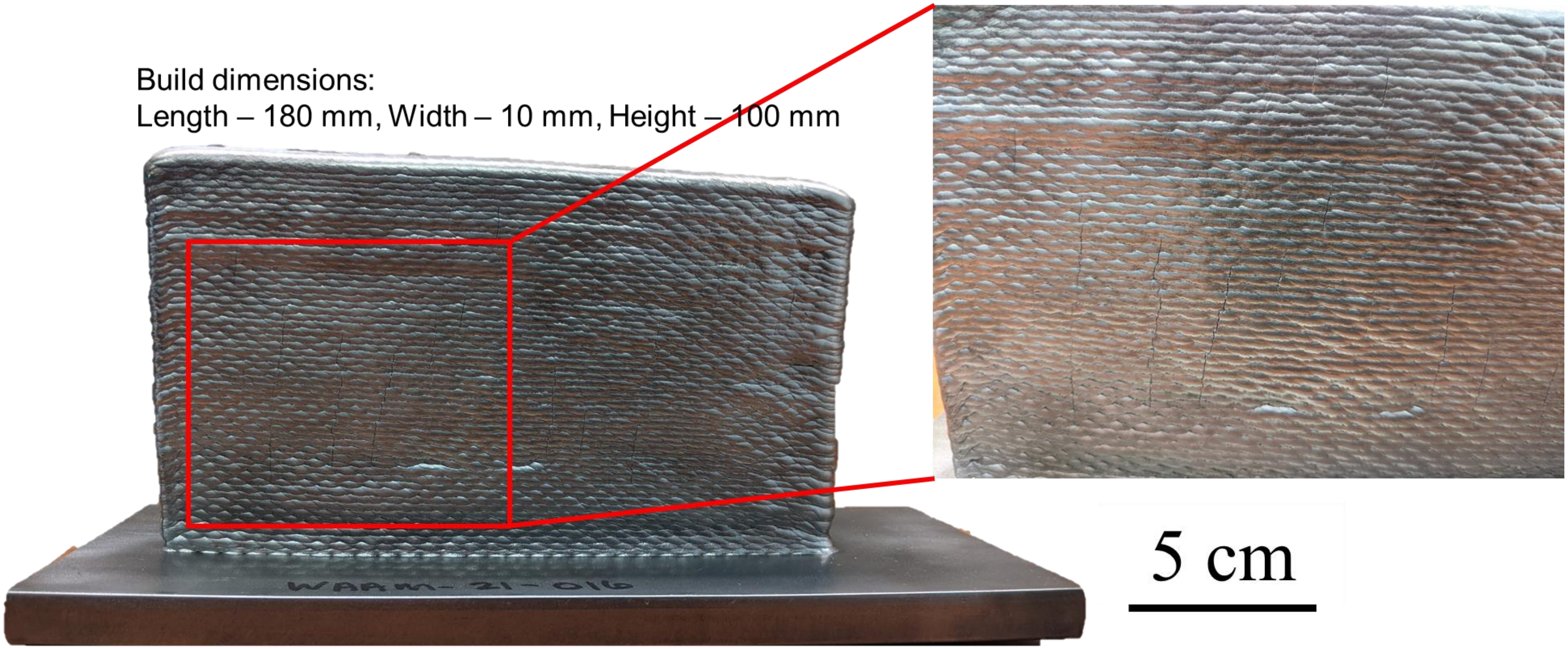
TCNI10

TCFE10



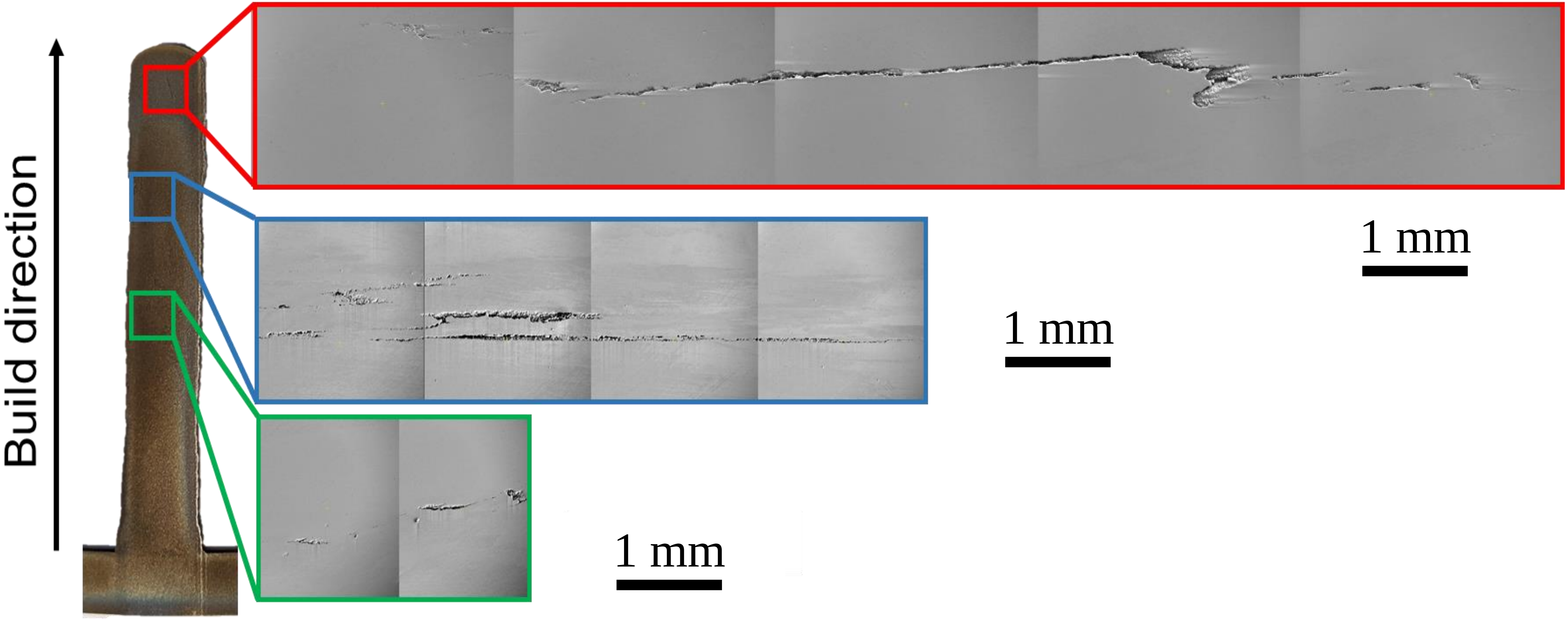
As-built 26 wt.% P91 graded alloy

Build dimensions:
Length – 180 mm, Width – 10 mm, Height – 100 mm



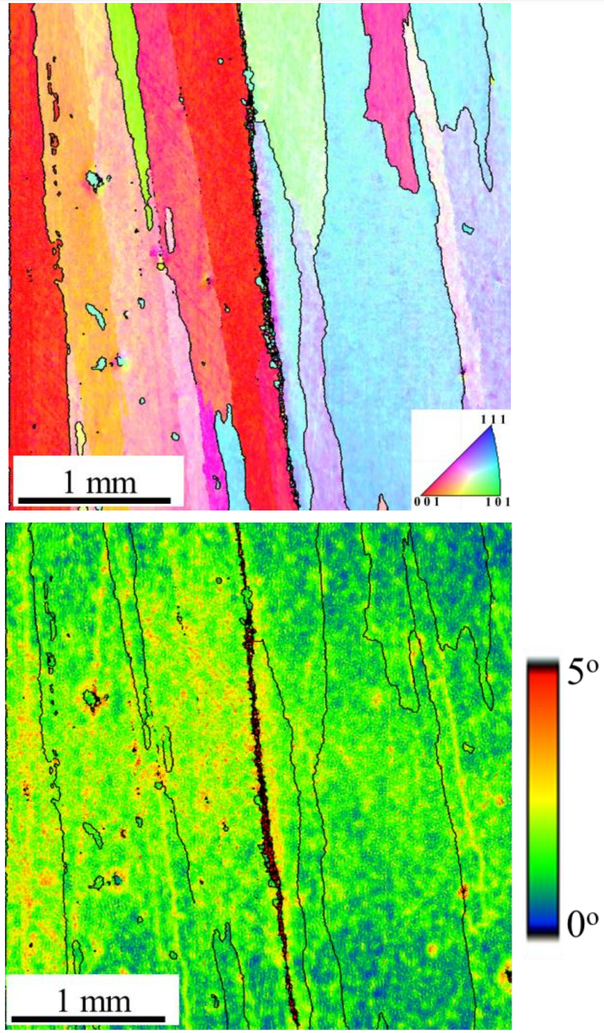
26 wt.% P91 build printed using WAAM showing the presence of surface cracks

As-built 26 wt.% P91 graded alloy

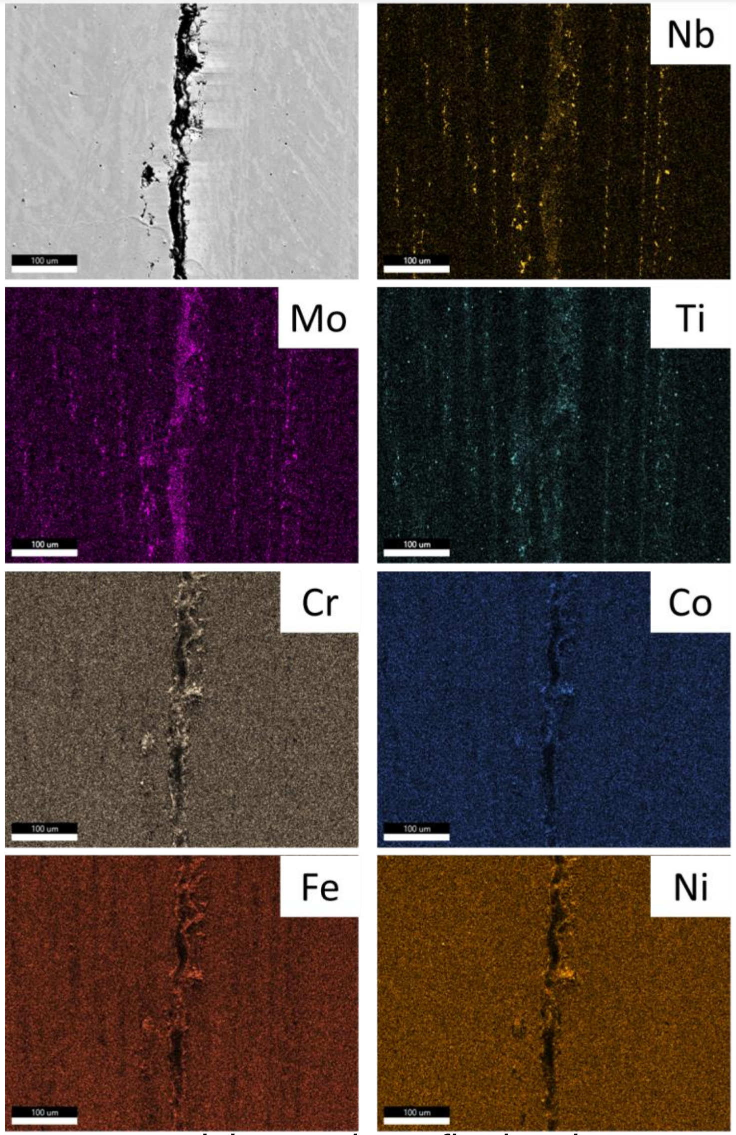


- No cracks found in the bottom portion and cracking starts after a certain height (~ 30 mm)
- Crack length increases as the height of the sample increases

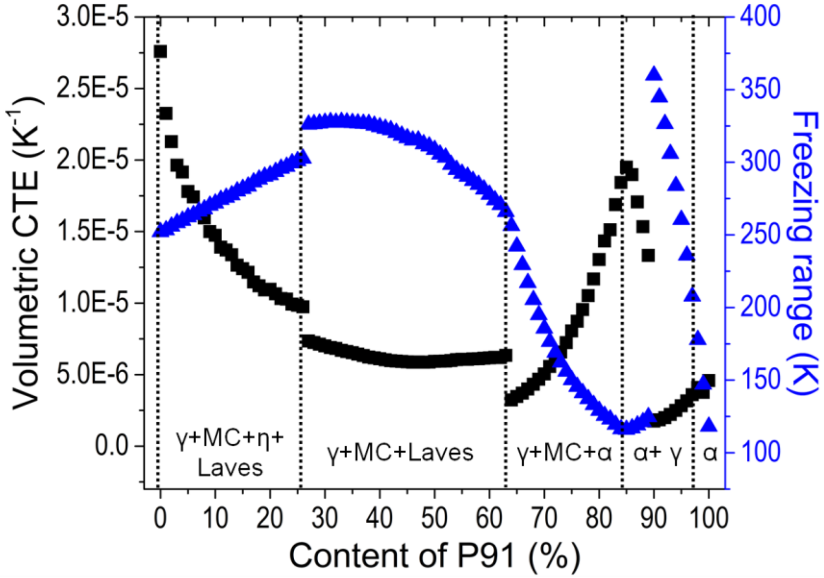
As-built 26 wt.% P91 graded alloy



IPF map confirming the crack to be intergranular and KAM map showing high stress regions near the crack



EDS maps around the crack confirming the presence of Laves phase through clusters of Nb, Ti and Mo



Scheil simulations for gradient compositions between P91 steel and 740H superalloy confirming the formation of Lave phase at 26 wt.% P91

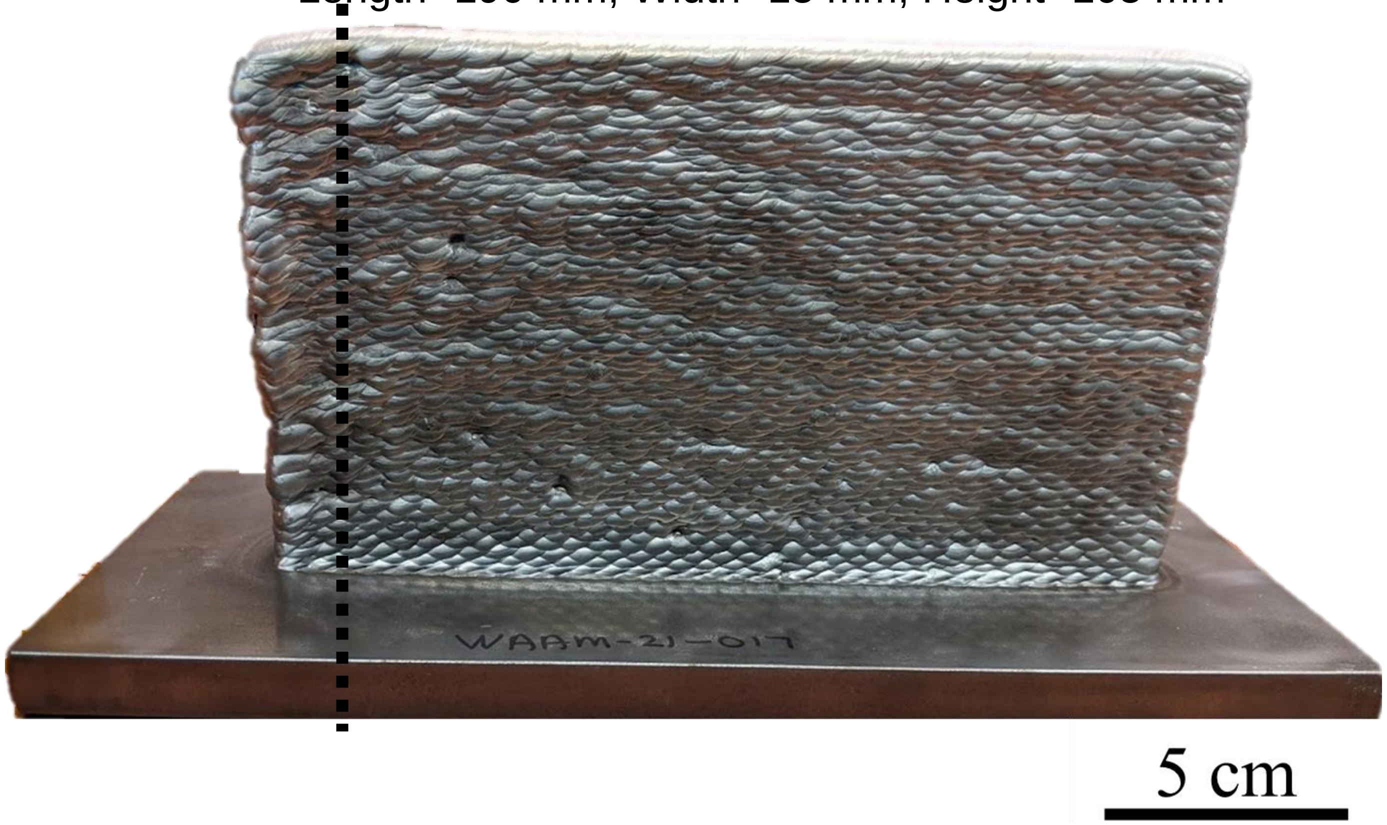
Cracks formed in 26 wt.% P91 build were found to be

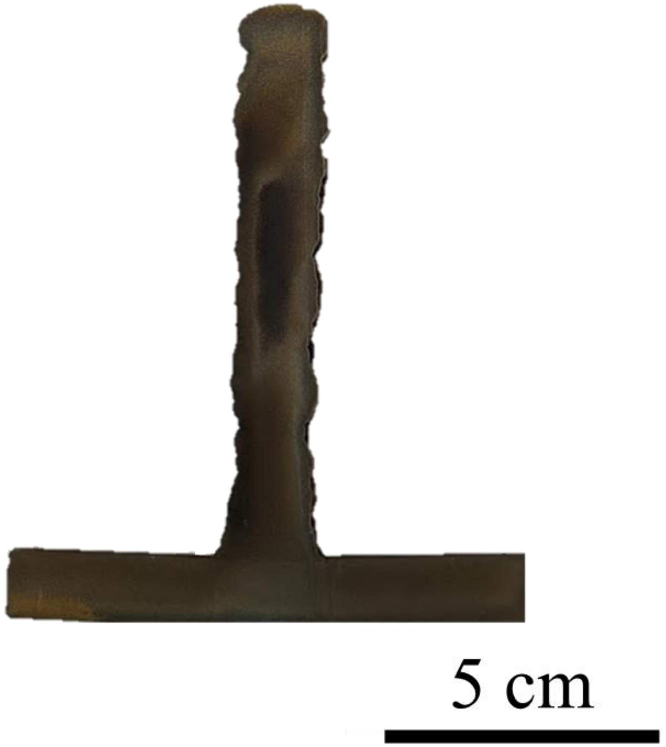
- Intergranular
- Surrounded by Laves phase

As-built 90 wt.% P91 graded alloy

Successful build without any cracks achieved

Build dimensions:
Length- 190 mm, Width- 15 mm, Height- 105 mm

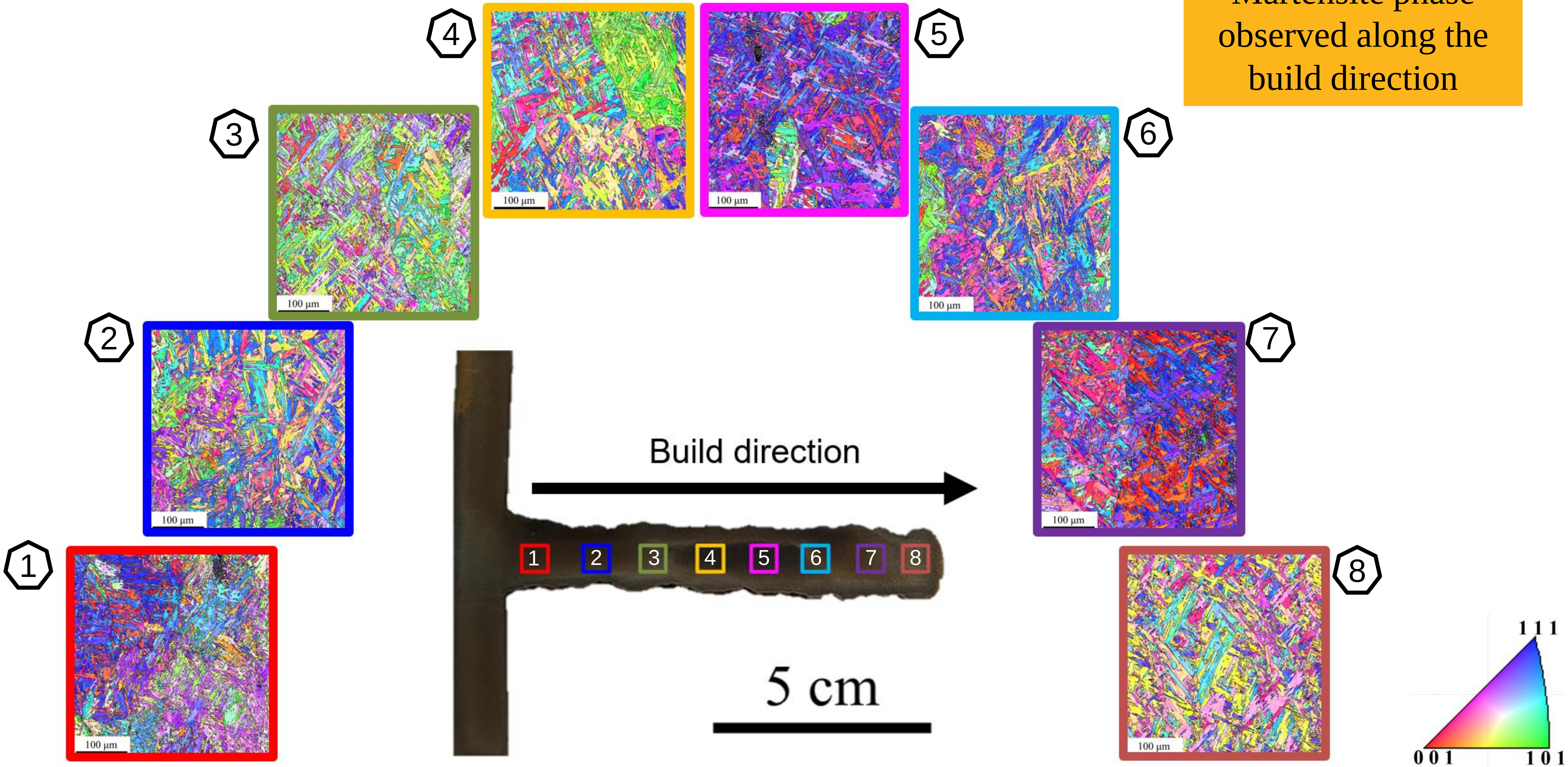




90 wt.% P91 build printed using WAAM and the sample extracted from the build for analysis

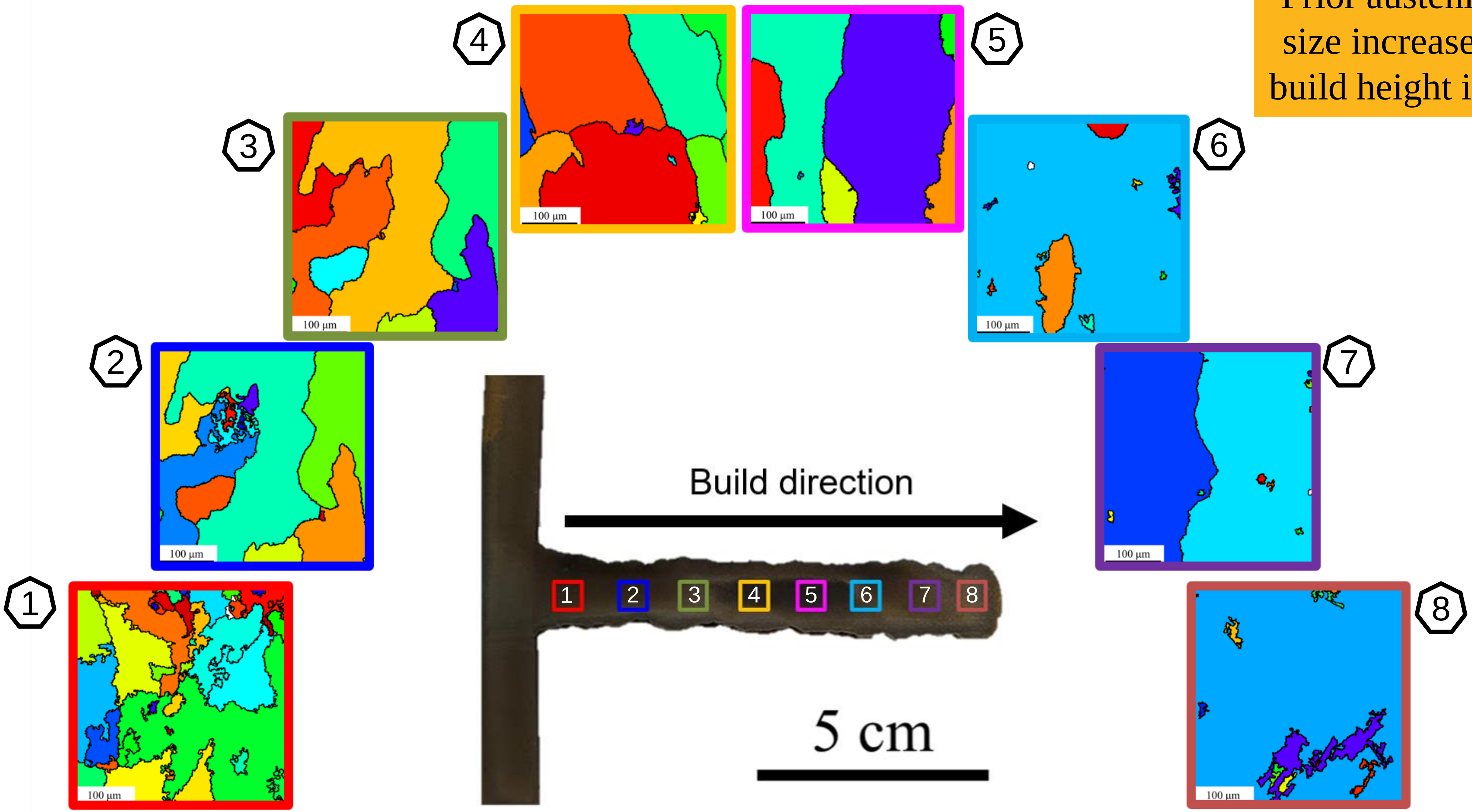
As-built 90 wt.% P91 graded alloy: EBSD – IPF image

Martensite phase observed along the build direction



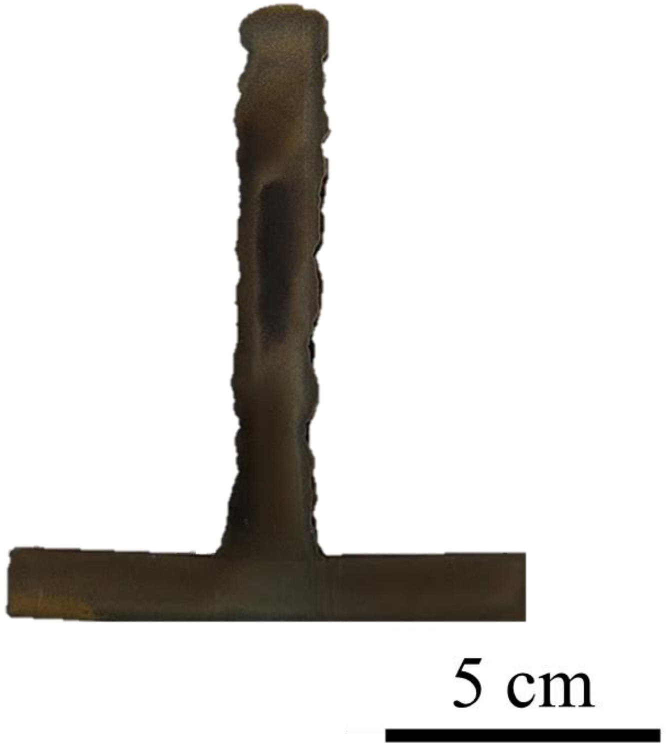
As-built 90 wt.% P91 graded alloy: Prior Austenite

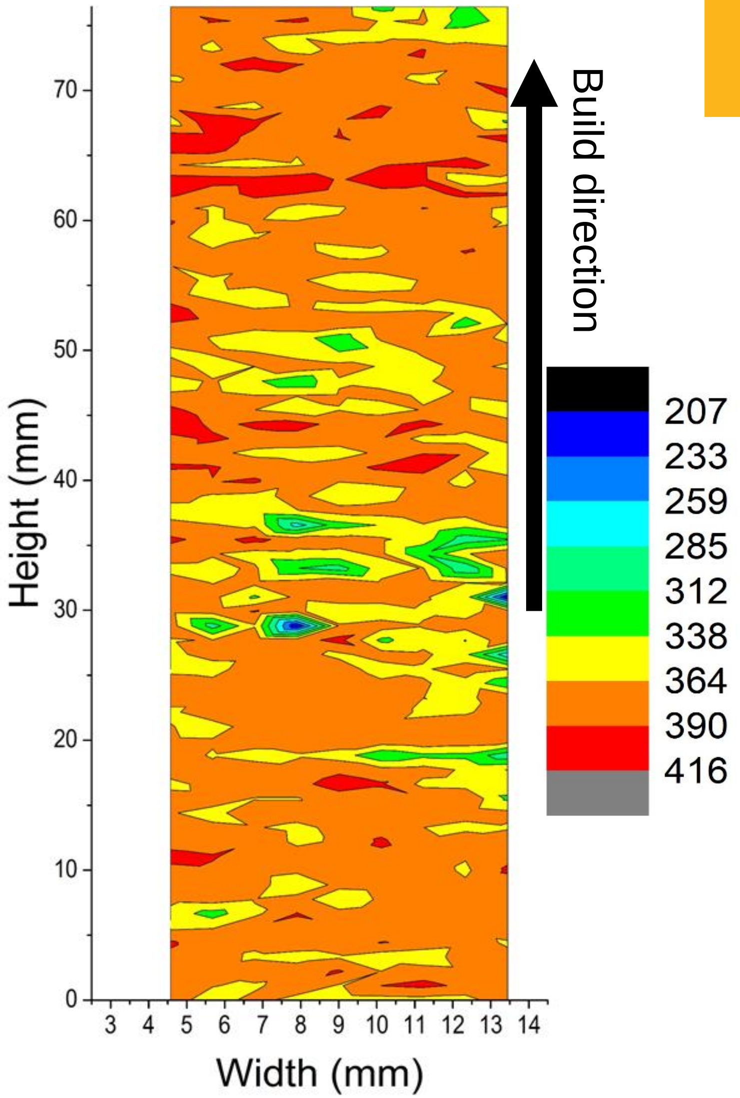
Prior austenite grain size increases as the build height increases



As-built 90 wt.% P91 graded alloy

Hardness variation predominantly uniform along the build direction





(5b) Interface structure design - 2nd Gen

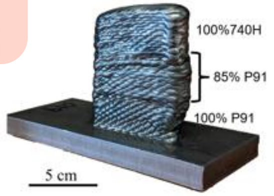
Design Roadmap

⑥ **3rd generation** printing and testing

⑤a Data driven ML and GA design for intermediate block **(2nd generation)**

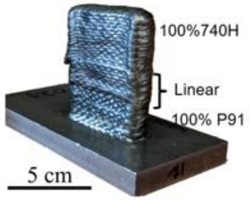
\+

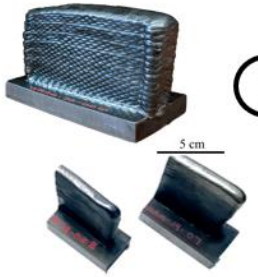
⑤b Interface structure design **(2nd generation)**



④ Post-heat treatment design on graded alloy builds **(1st generation)**

③ Computational design on intermediate blocks





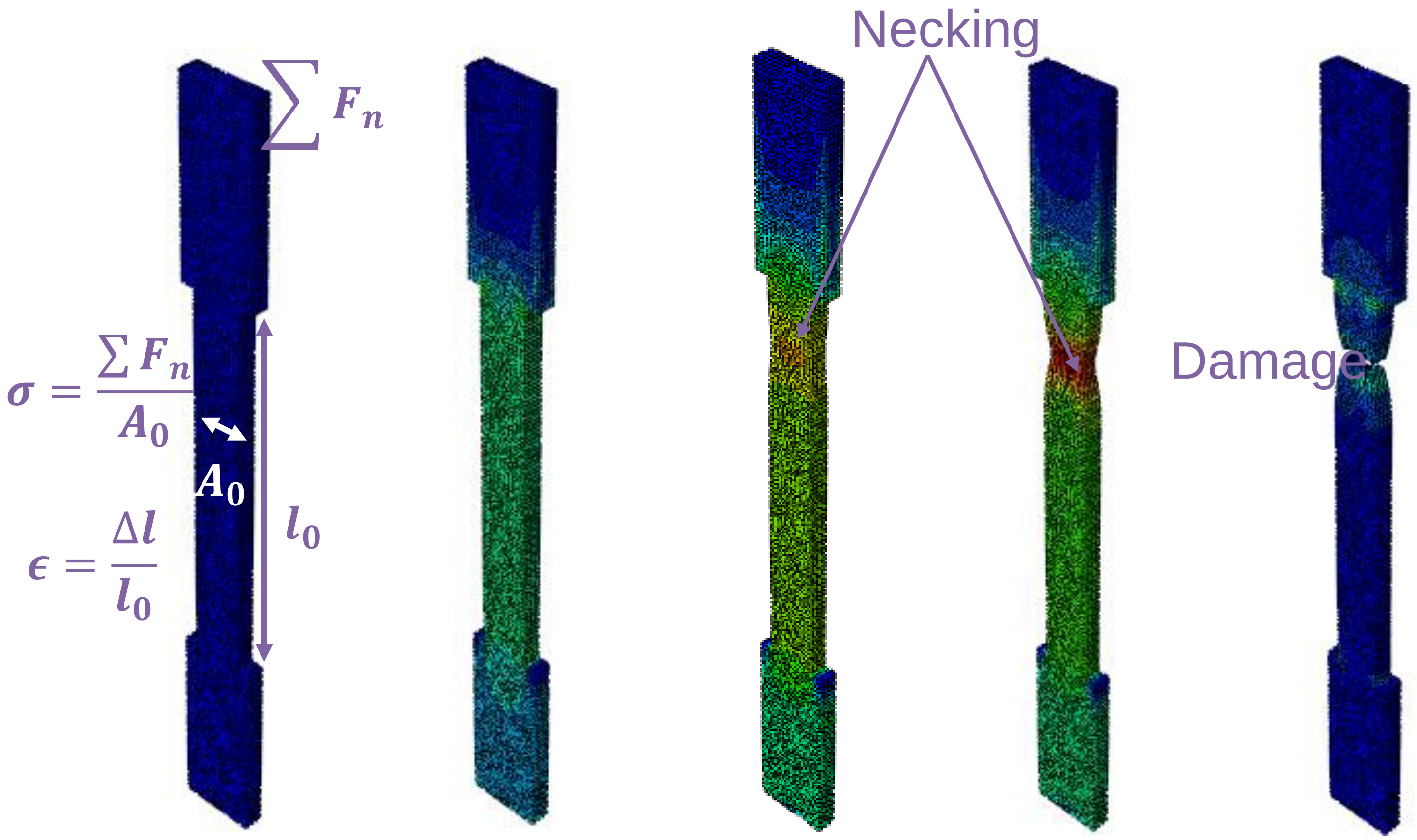
① Inconel 740H & P91 printing and post-heat treatment

② Sharp interface builds for deposition sequence and post-heat treatment

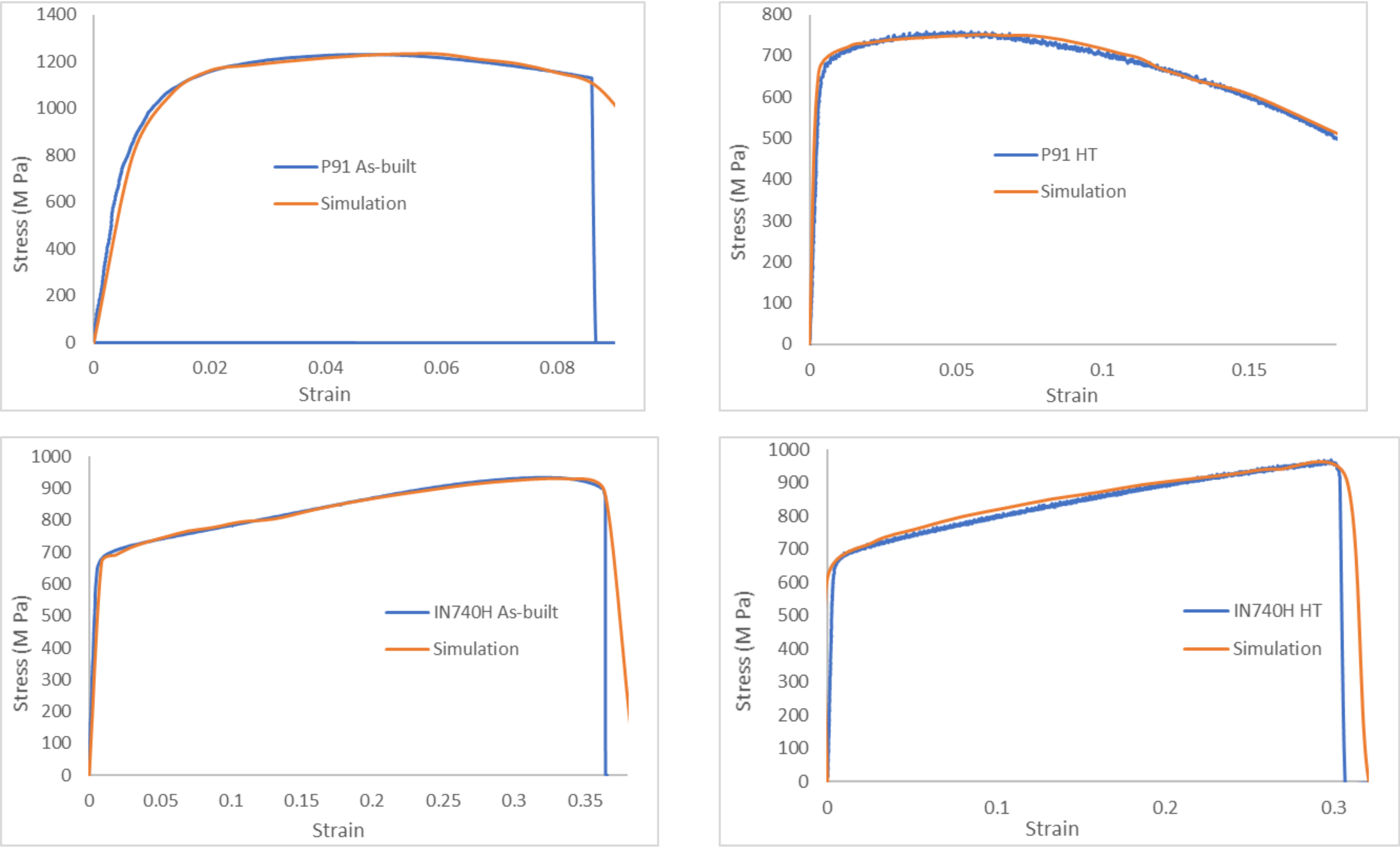
Tensile test modeling

- Ductile damage model developed to simulate tensile failure
- Phenomenological model for predicting the onset of damage due to nucleation, growth, and coalescence of voids
- Describes the rate of degradation of the material stiffness once the corresponding initiation criterion has been reached

- By default, an element is removed from the mesh if all the section points at any one integration location have lost their load-carrying capacity

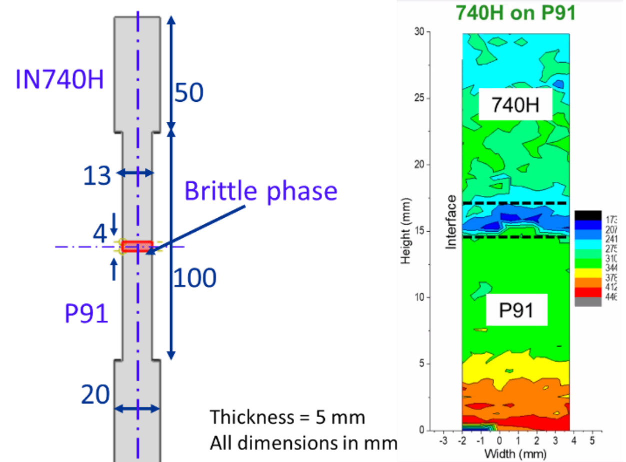


Model calibration

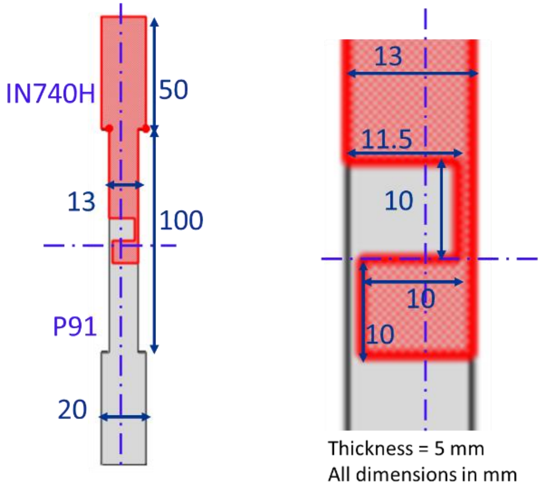


JC hardening law $\bar{\sigma} = \left[A + B\left(\bar{\varepsilon}^{pl}\right)^{n}\right]$

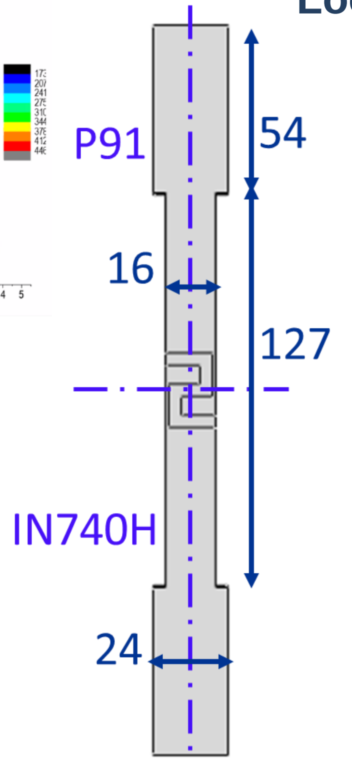
Design comparison



Sharp interface



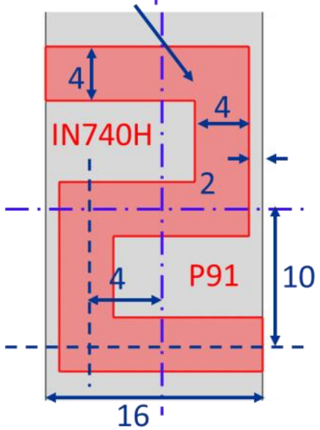
Interface_1



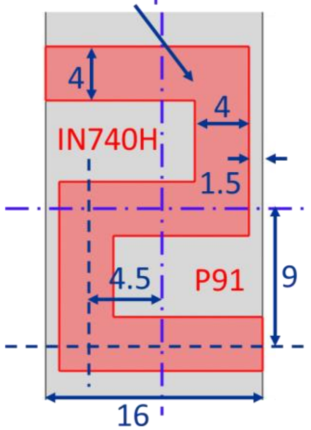
- No improvement between **LockingInterface_1** and **LockingInterface_3**

Increase of IN740H area/material on side improves ductility

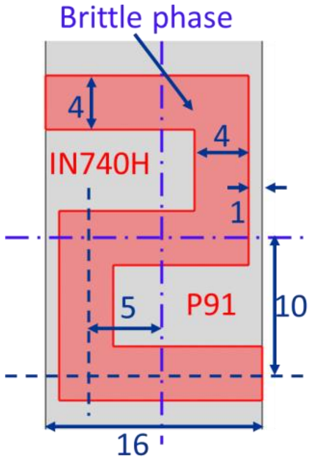
LockingInterface_3

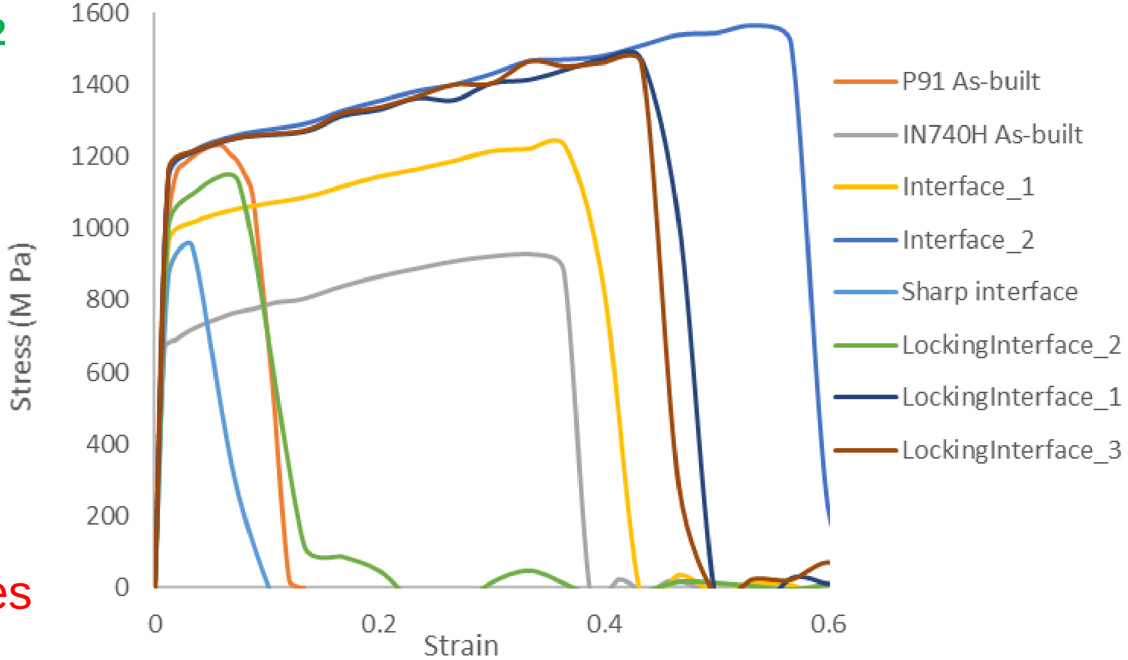


LockingInterface_1



LockingInterface_2

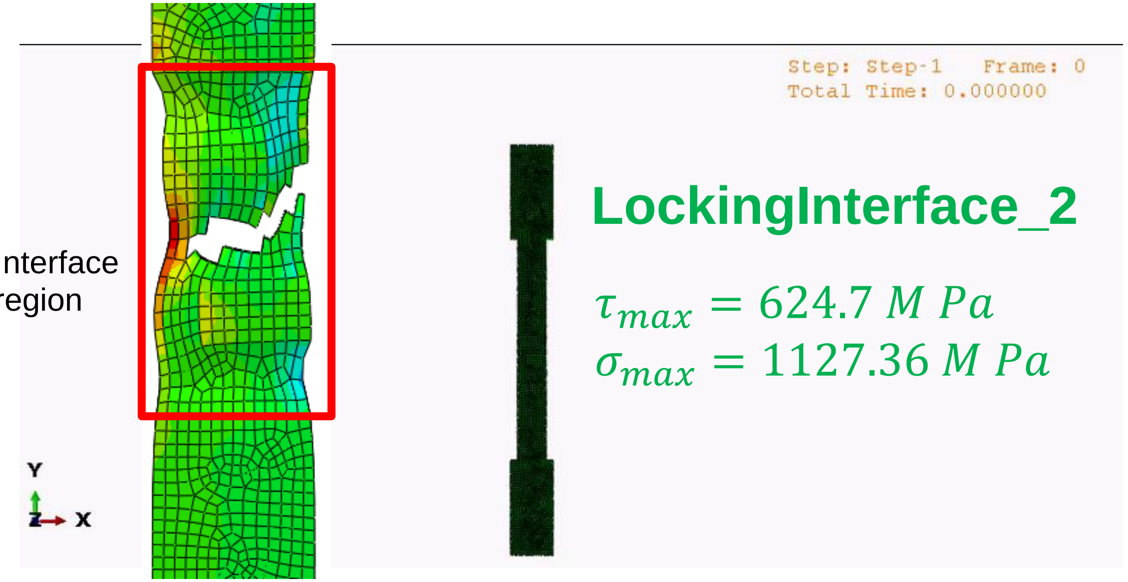




Brittle phase property dominates

Design comparison: Failure

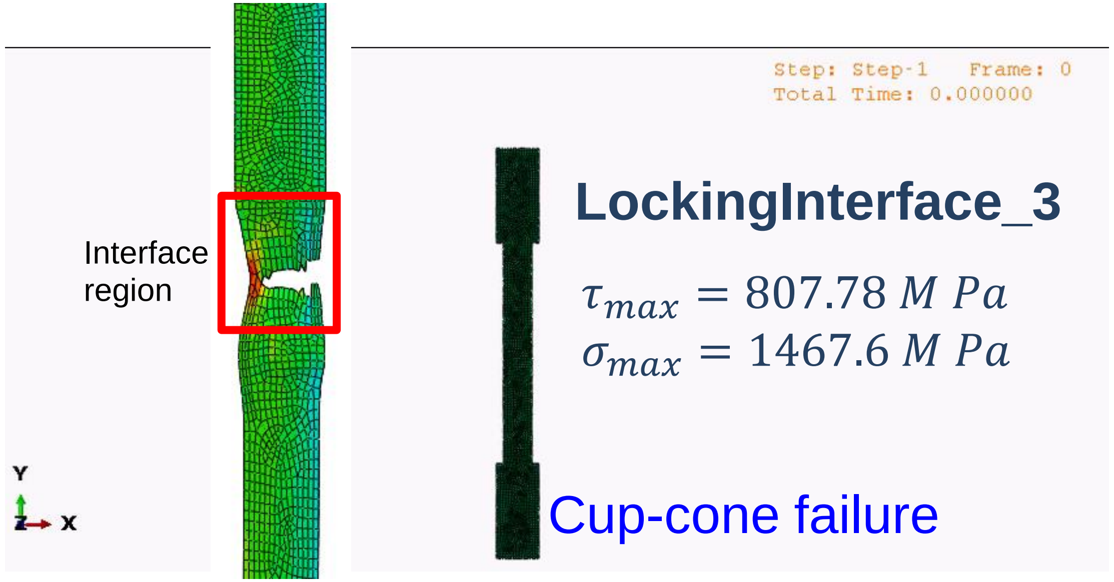
Interface region



LockingInterface_2

$$\tau_{max} = 624.7\ MPa$$
$$\sigma_{max} = 1127.36\ MPa$$

Interface region



LockingInterface_3

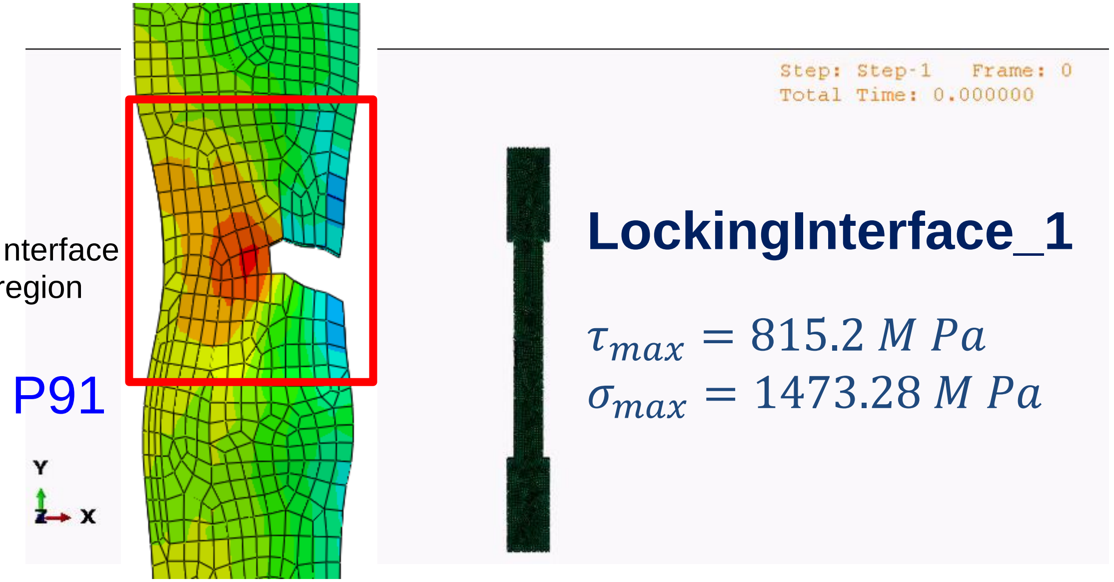
$$\tau_{max} = 807.78\ MPa$$
$$\sigma_{max} = 1467.6\ MPa$$

Cup-cone failure

- Both LockingInterface_1 and 3 show more plastic deformation in the IN740H region (lower portion) compared to LockingInterface_2

Damage initiates in P91

Interface region

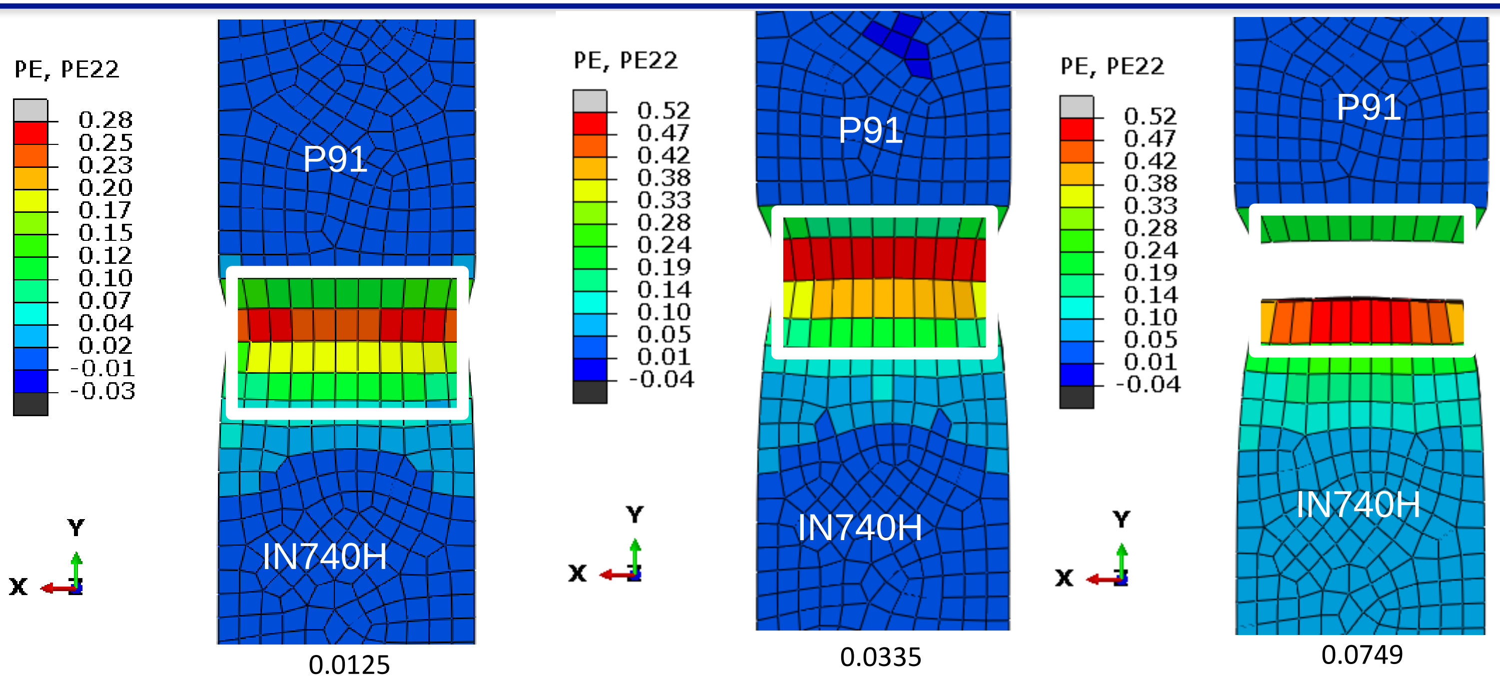


LockingInterface_1

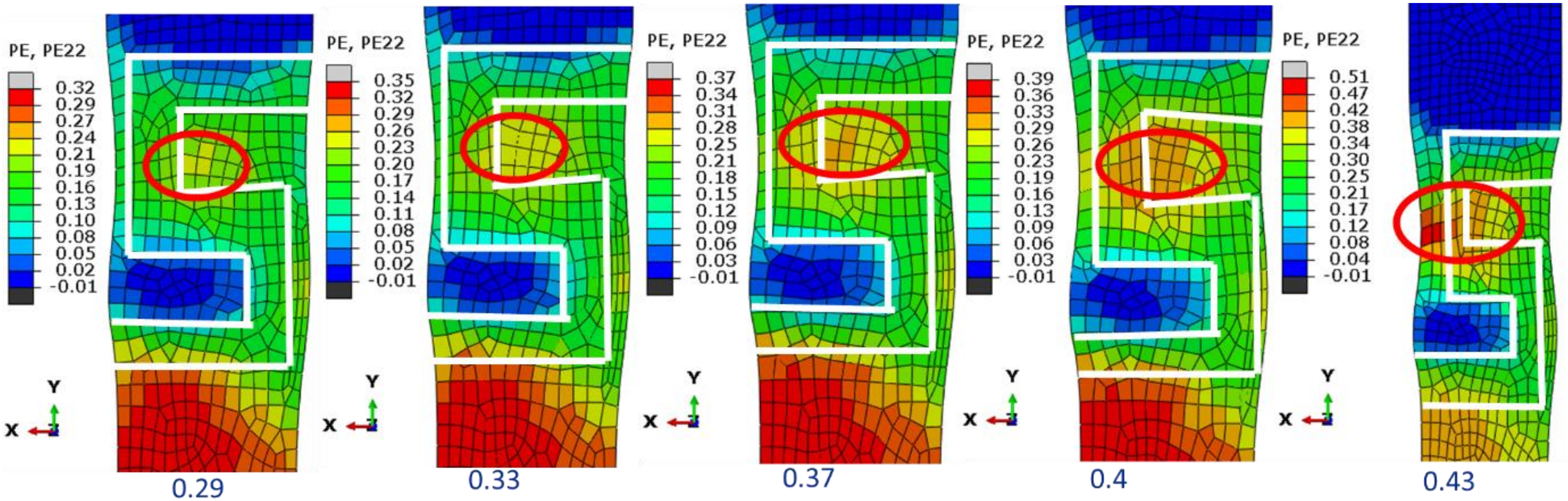
$$\tau_{max} = 815.2\ MPa$$
$$\sigma_{max} = 1473.28\ MPa$$

Deformation comparison

For sharp interface, load distributes to nearby interface elements and early failure occurs due to reduced ultimate strength in brittle phase compared to P91



By introducing locking design load gradually transfers from IN740H to Brittle phase to P91

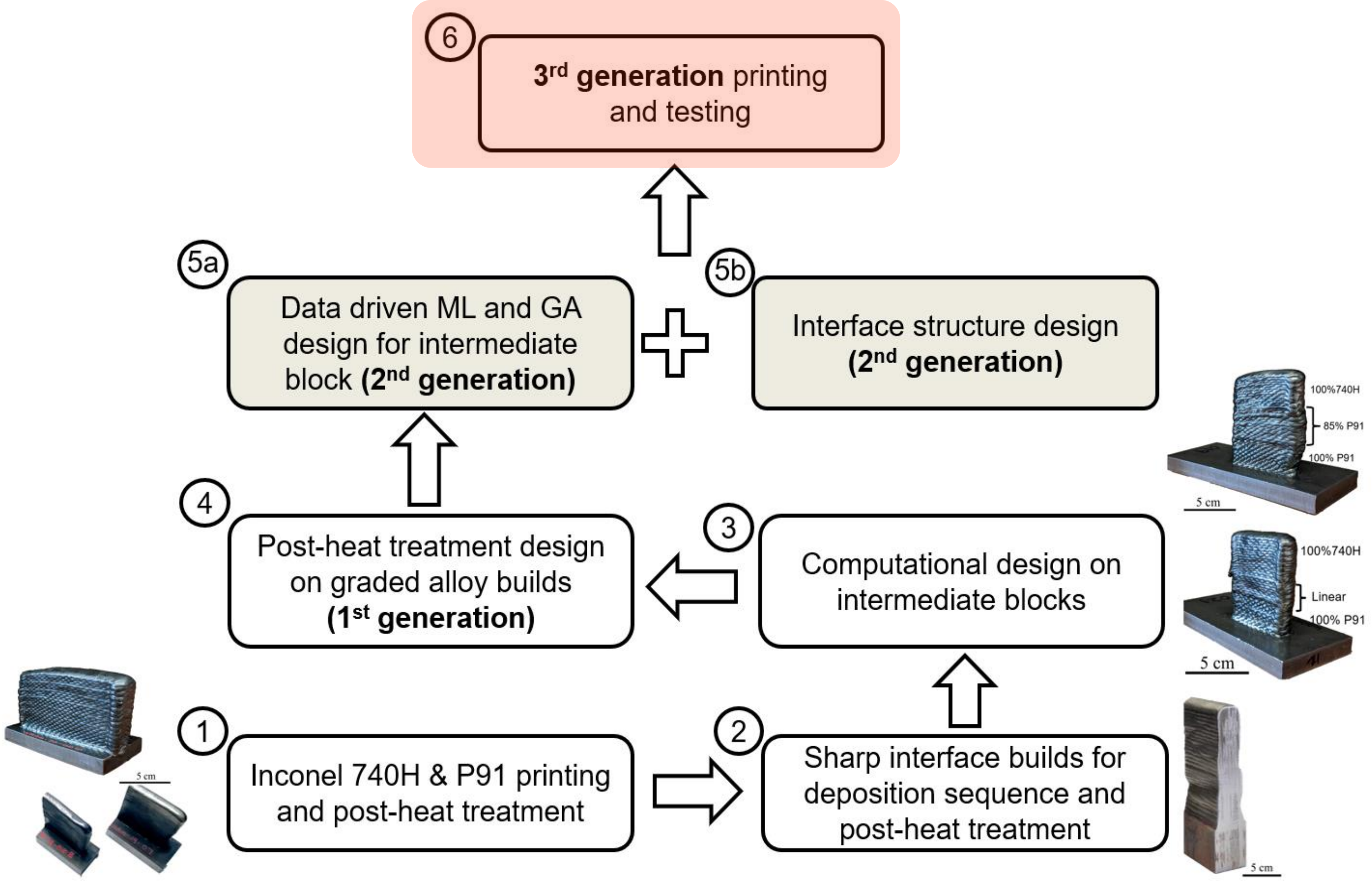


Summary

- Non-standard ASTM tensile bar designs were studied
- Locking structure design introduced in the interface zone
- Locking interface 3 shows promise w.r.t strength and printability

Future work

- More performance evaluation are undergoing.
- Gen 3 build with mechanical testing will be performed.



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