NIST Diffusion Workshop, Apr. 14-15, 2026

Understanding microstructure evolution in additively manufactured alloys during heat treatment



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Acknowledgements:
Yunhao Zhao, Xin Wang,
Soumya Sridar, Luis Pizano, Chantal Sudbrack









University of Pittsburgh

Introduction of Inconel 718

Typical Composition

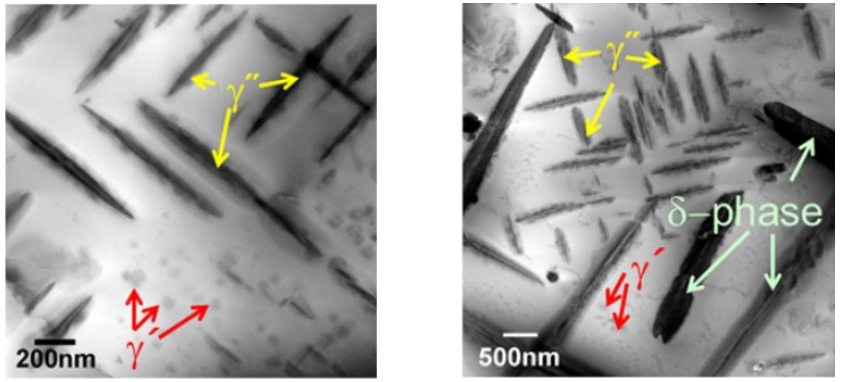
Inconel 718	Ni	Fe	Cr	Nb	Mo	Ti	Al	C
Comp. (wt.%)	Bal.	19.35	19.00	5.125	3.050	0.90	0.50	0.035
Comp. (at.%)	Bal.	20.00	21.17	3.2	1.84	1.09	1.07	0.00169

Major Phases

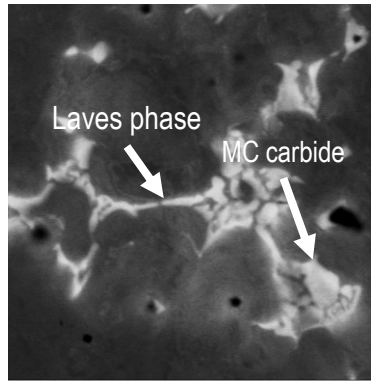
δ and γ′ are stable, but γ″ is metastable

Phase	Crystal structure	Formula	Comments
γ	FCC (disordered A1)	Ni-rich with other elements	matrix
γ′	FCC (ordered $L1_2$)	$(Ni)_3(Al,Ti)$	strengthening
γ″	BCT (ordered $D0_{22}$)	Ni_3Nb	Principal strengthening metastable
δ	Orthorhombic (ordered Cu_3Ti-type)	Ni_3Nb	detrimental
MC	Cubic	(Ti, Nb)C	-
Laves	Hexagonal (C14)	$(Ni,Fe,Cr)_2(Nb,Ti,Mo)_1$	detrimental

γ', γ", and δ (STEM) [2016Sam]

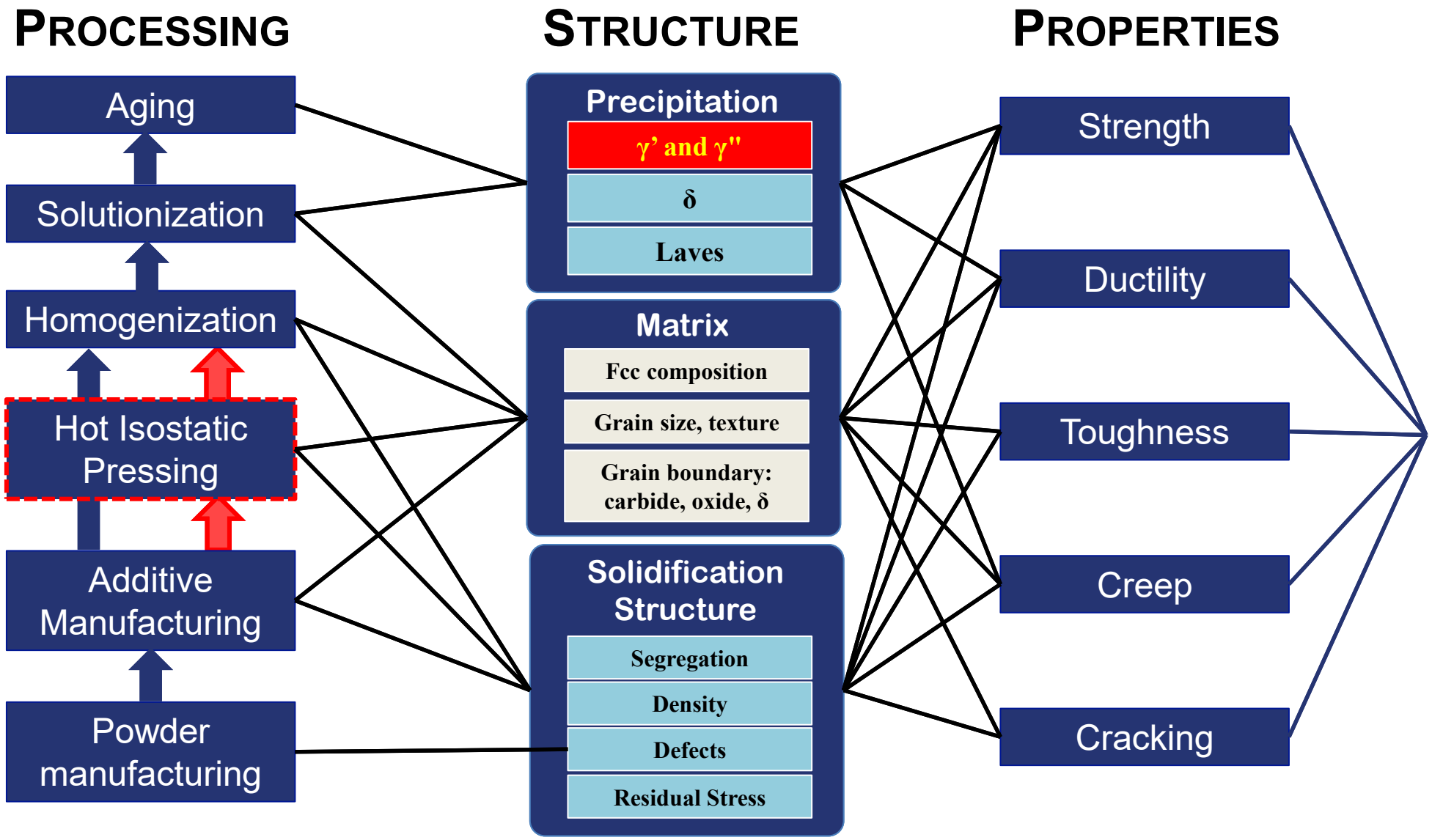


MC carbide and Laves phase (SEM, this work)



[2016Sam] Sames W J, Unocic K A, Dehoff R R, et al. Thermal effects on microstructural heterogeneity of Inconel 718 materials fabricated by electron beam melting[J]. Journal of Materials Research, 2014, 29(17): 1920-1930.

Systems design chart of Inconel 718

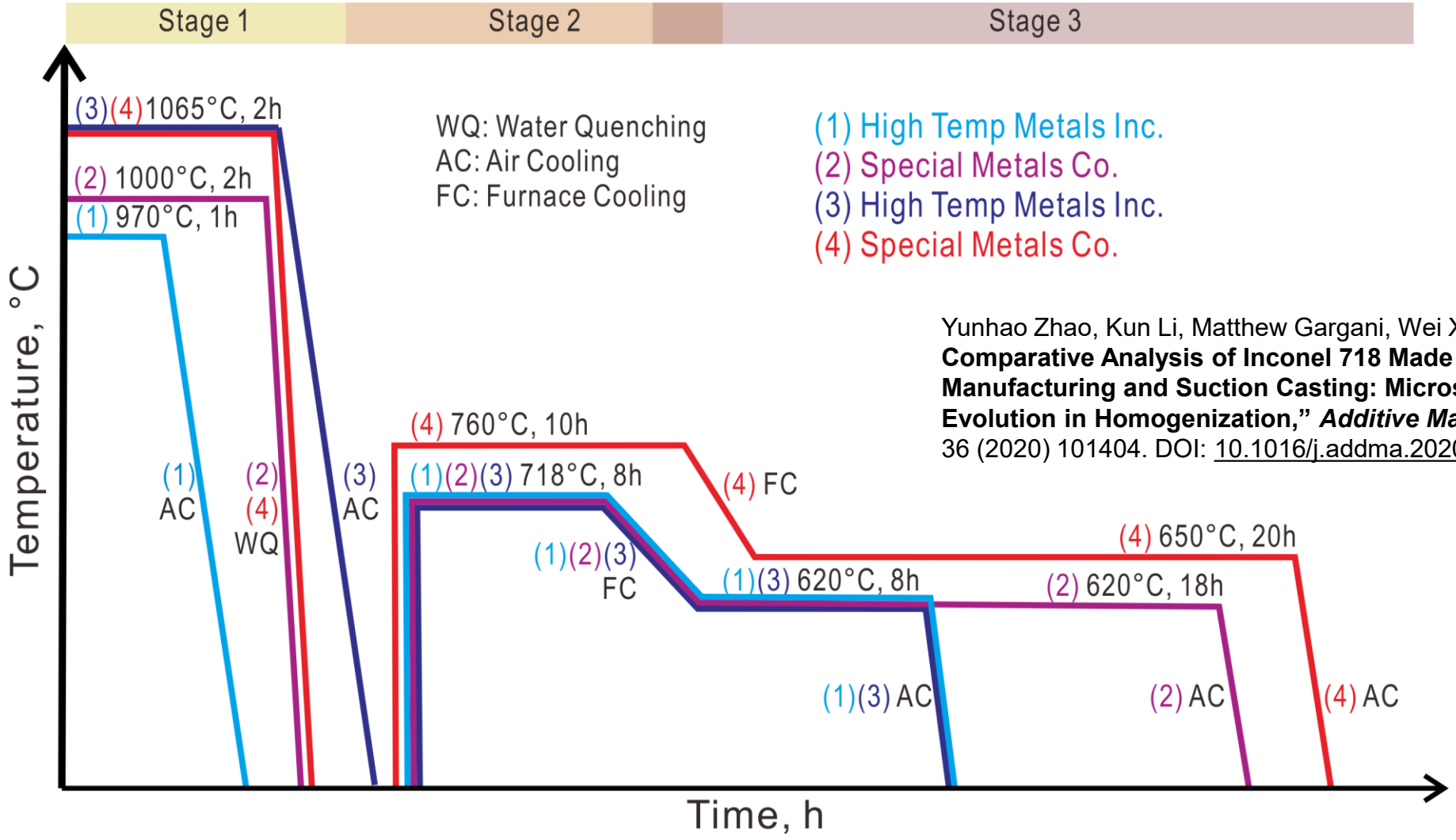


Heat treatment diagram of Inconel 718

Stage 1-Homogenization (normalizing): remove segregation and detrimental Laves and δ phases.

Stage 2-aging at around 718°C: promoting precipitation of the γ'' phase.

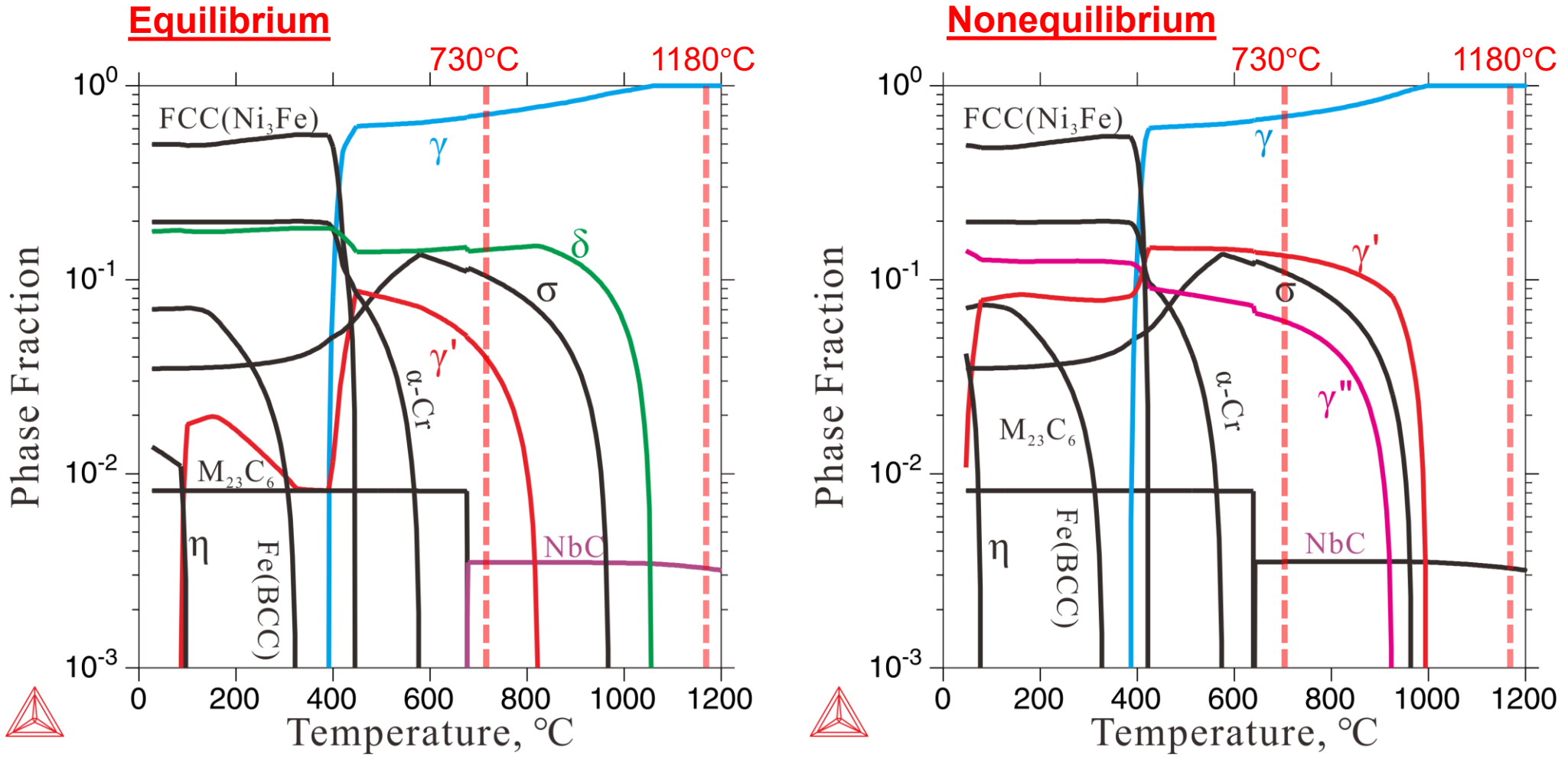
Stage 3-aging at around 620°C: promoting precipitation of the γ' phase.



Yunhao Zhao, Kun Li, Matthew Gargani, Wei Xiong, **"A Comparative Analysis of Inconel 718 Made by Additive Manufacturing and Suction Casting: Microstructure Evolution in Homogenization,"** ***Additive Manufacturing***, 36 (2020) 101404. DOI: 10.1016/j.addma.2020.101404

Step (phase) diagram of Inconel 718

In this work, **1180°C** is selected as the homogenization temperature to obtain pure γ and MC phases

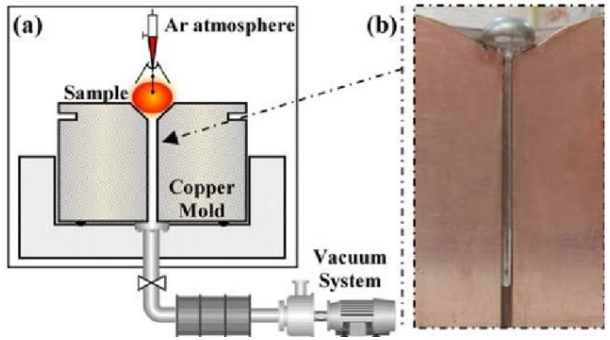


Yunhao Zhao, Kun Li, Matthew Gargani, Wei Xiong, **"A Comparative Analysis of Inconel 718 Made by Additive Manufacturing and Suction Casting: Microstructure Evolution in Homogenization,"** ***Additive Manufacturing***, 36 (2020) 101404. DOI: 10.1016/j.addma.2020.101404

Suction Casting vs. Additive Manufacturing



Suction casting

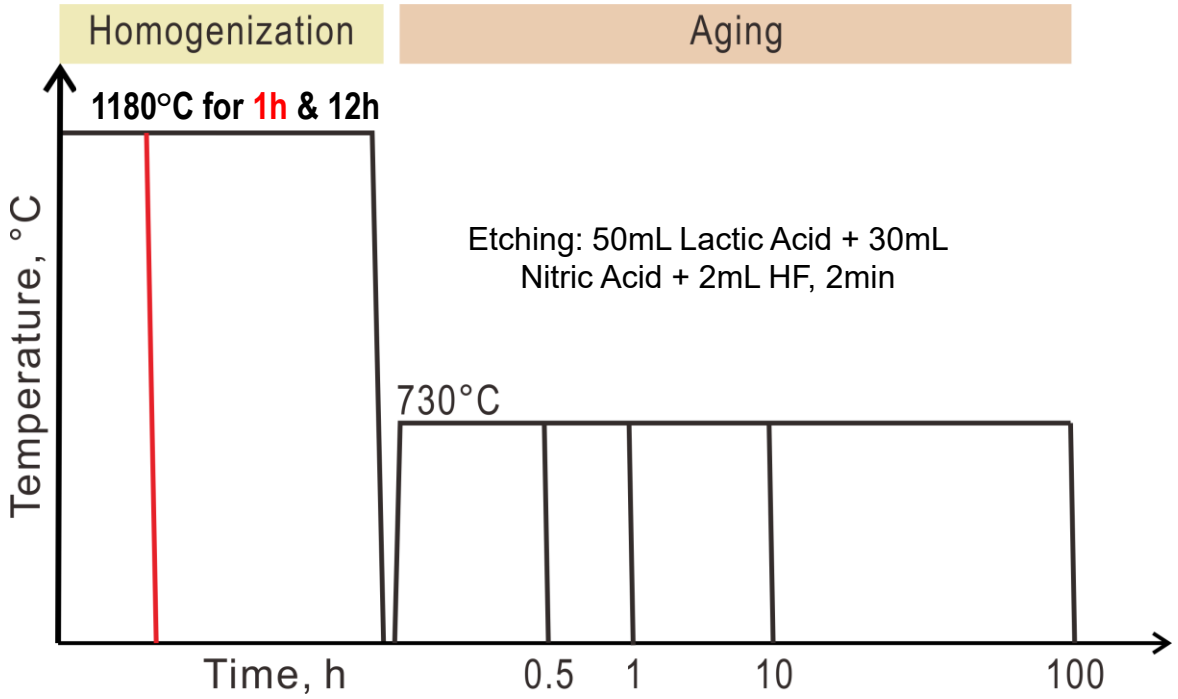






EOS powder-bed laser melting

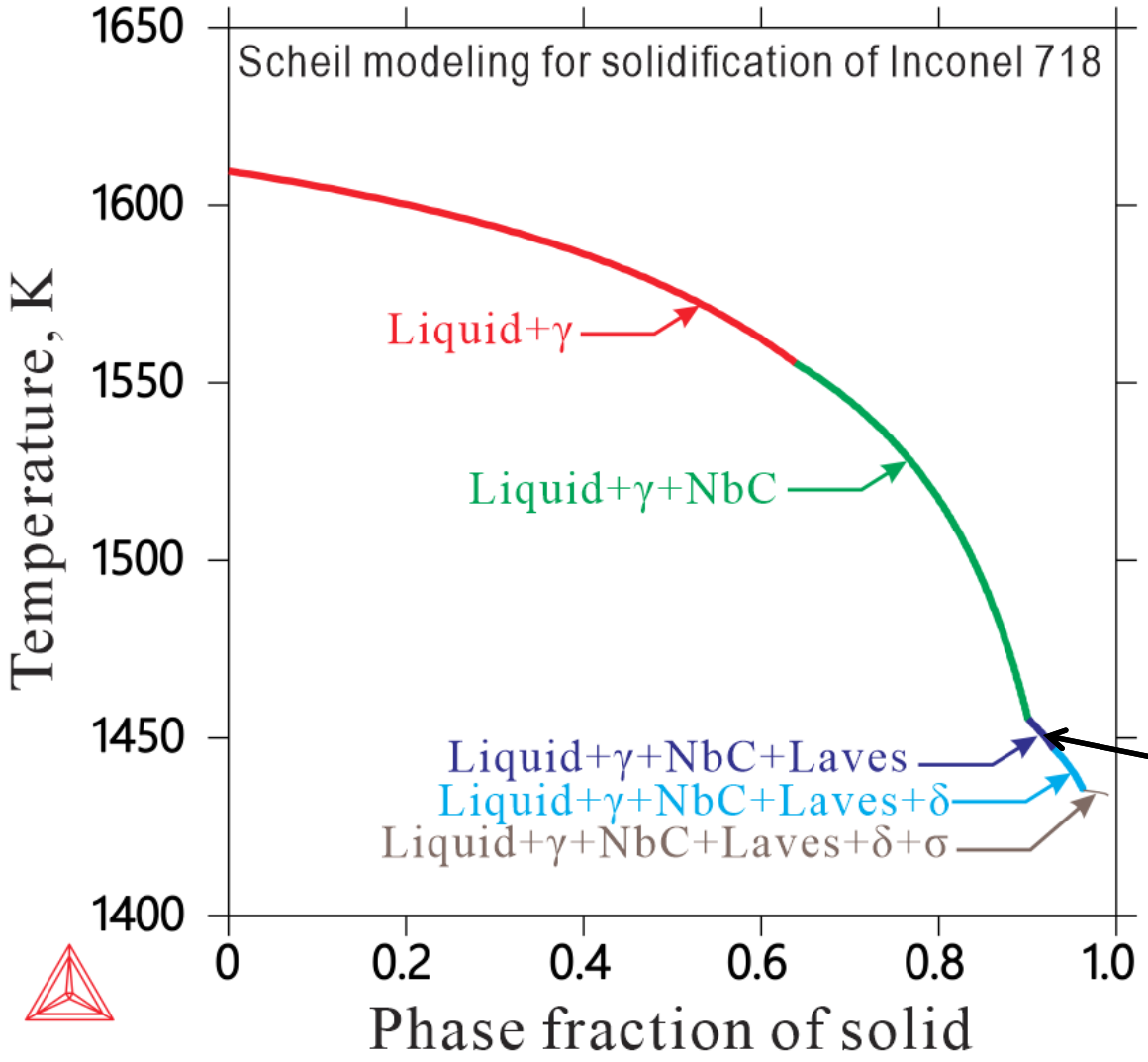
1) Homogenization heat treatment
   - ➢1180°C for 1 h
   - ➢1180°C for 12 h
2) Aging heat treatment
   - ➢730°C for 0.5h, 1h, 10h, and 100h
   - ➢Water quench



Sample heat treatment diagram in this work

Ref for suction casting: Ziya Ozgur Yazici et al., 2016. DOI: 10.1007/s12540-016-5220-9

Scheil modeling of solidification



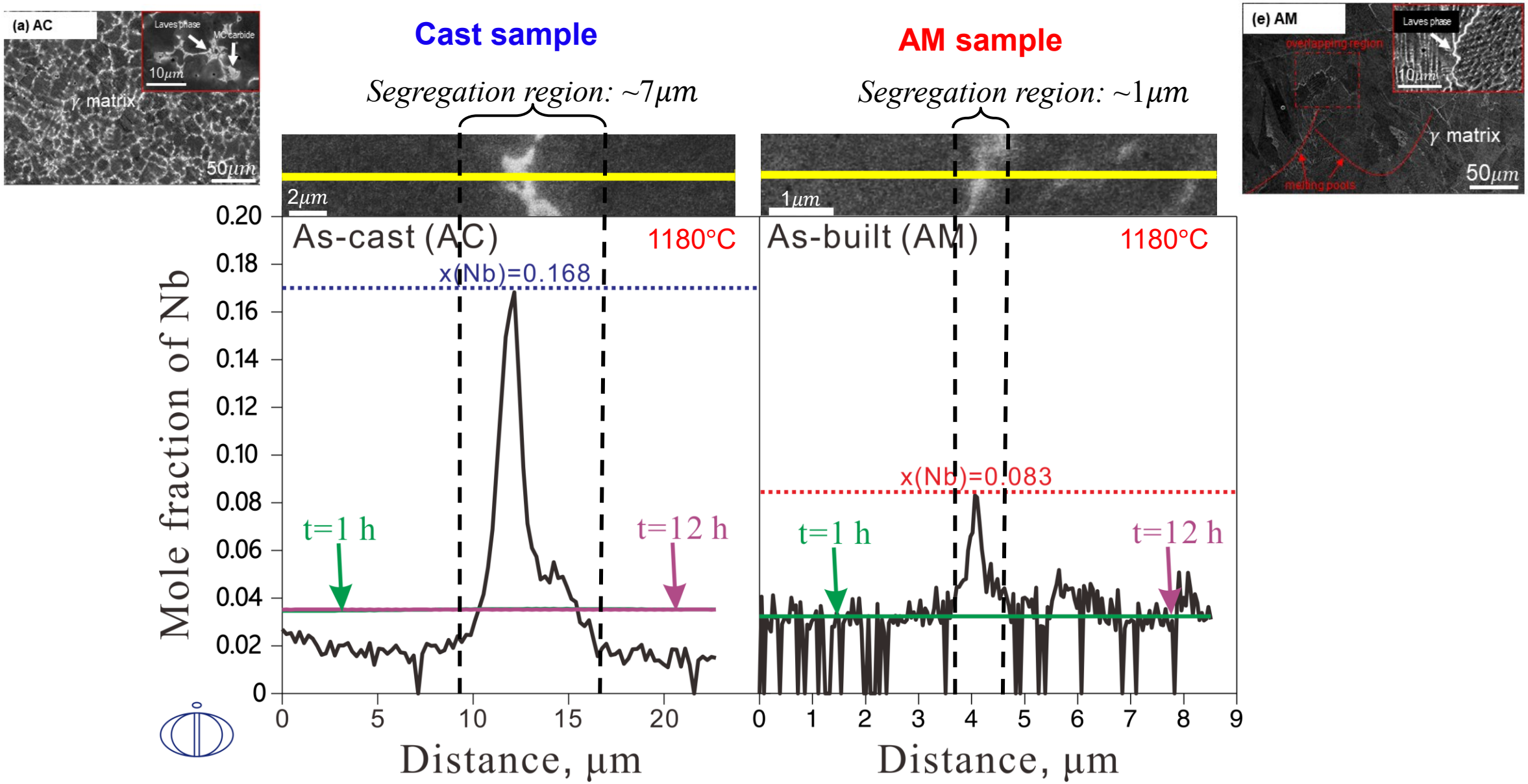
Phase in solidification

Phase	Crystal structure	Formula
γ	FCC (disordered A1)	Ni-base with Nb
NbC	Cubic	NbC
δ	Orthorhombic (ordered Cu_3Ti-type)	Ni_3Nb
Laves	Hexagonal (C14)	$(Ni,Fe,Cr)_2(Nb,Ti,Mo)_1$
σ	Tetragonal	Cr, Fe, Mo

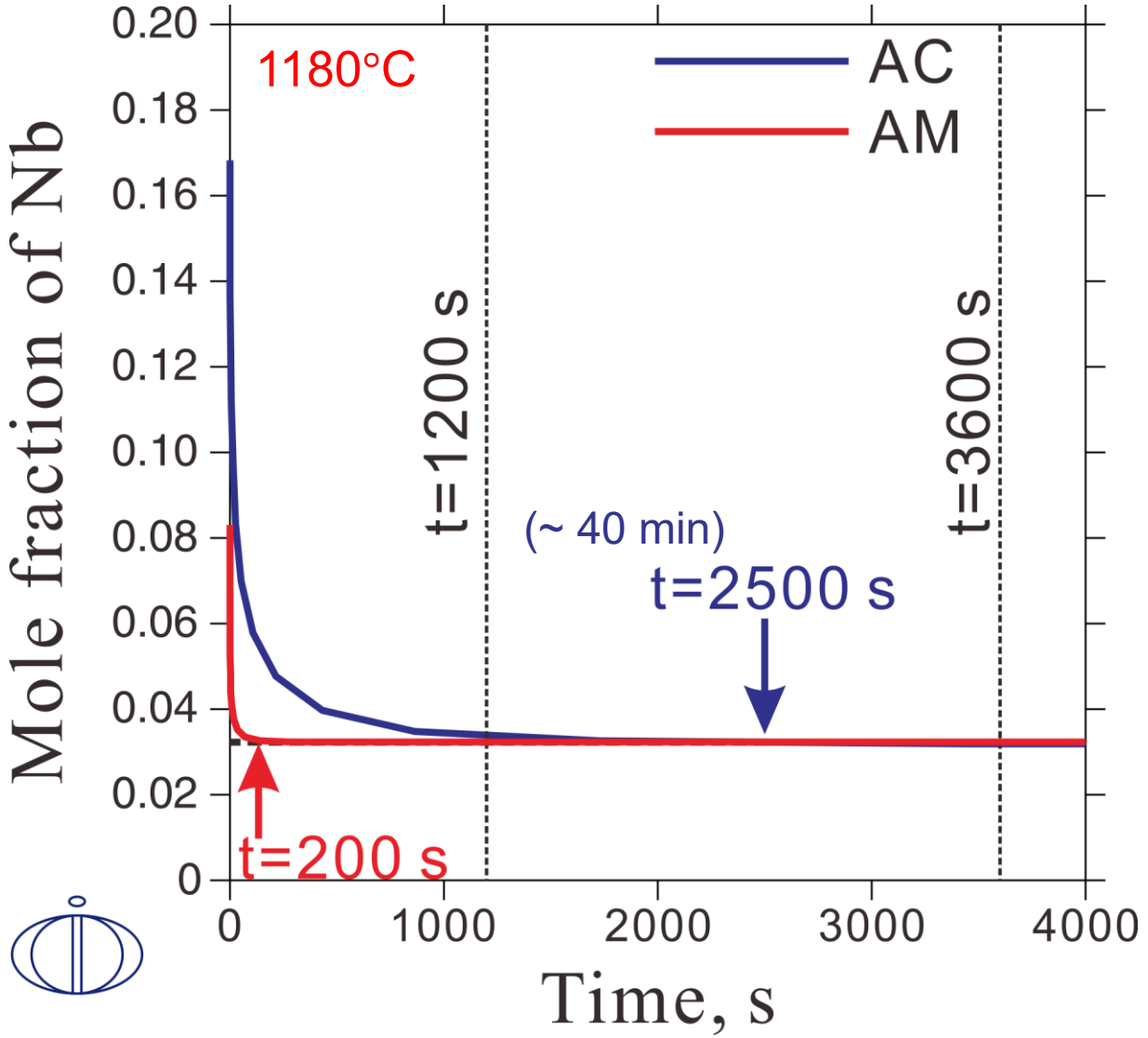
Laves_C14 will form during solidification

Yunhao Zhao, Kun Li, Matthew Gargani, Wei Xiong, **"A Comparative Analysis of Inconel 718 Made by Additive Manufacturing and Suction Casting: Microstructure Evolution in Homogenization,"** ***Additive Manufacturing***, 36 (2020) 101404. DOI: 10.1016/j.addma.2020.101404

DICTRA simulation for homogenization



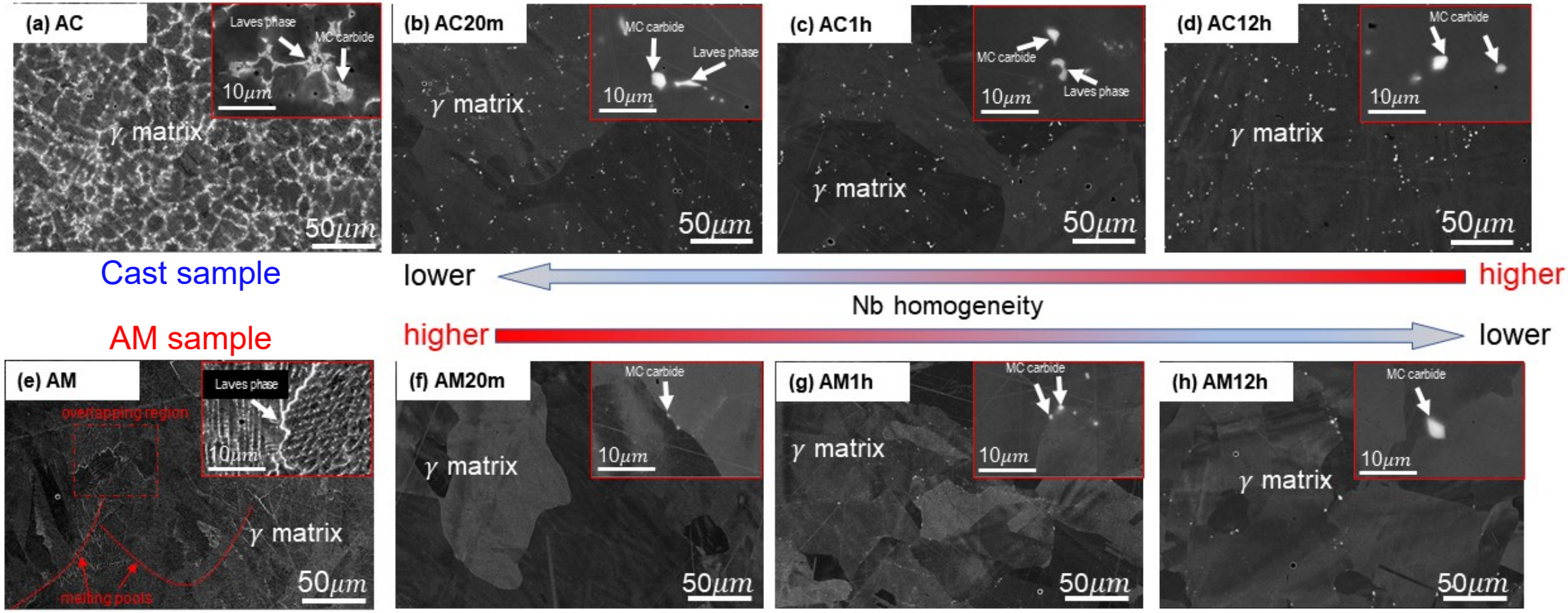
DICTRA simulation for homogenization



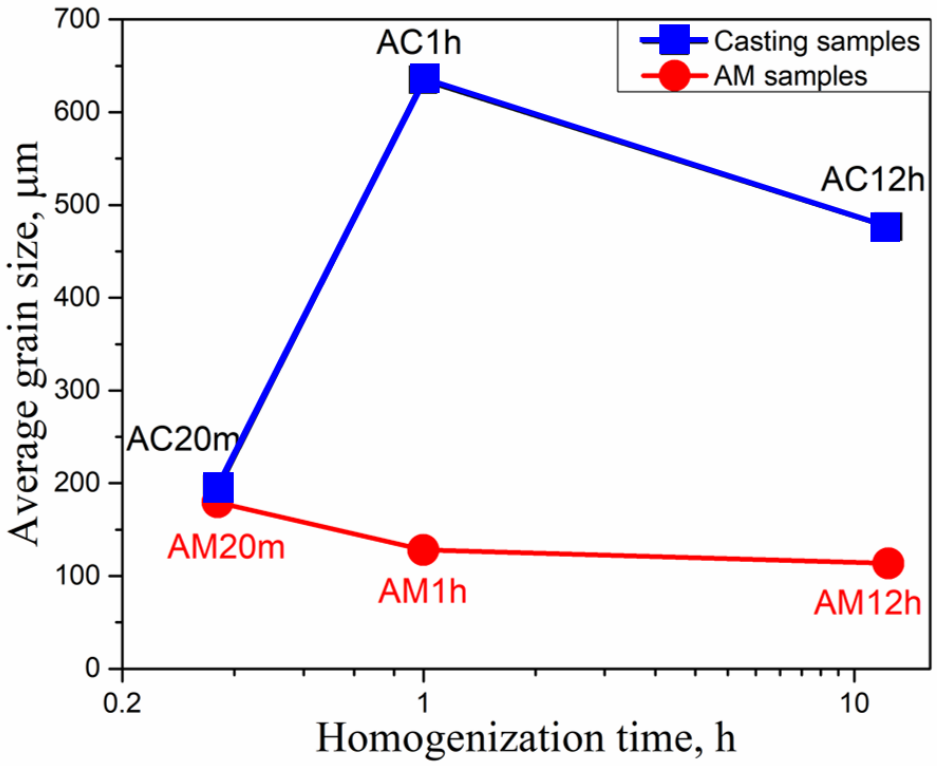
Soumya Sridar, Yunhao Zhao, Wei Xiong, **"Phase Transformations during Homogenization of Inconel 718 Alloy Fabricated by Suction Casting and Laser Powder Bed Fusion: a CALPHAD case study evaluating different homogenization models,"** ***Journal of Phase Equilibria and Diffusion***, 42 (2021) 28–41. DOI: 10.1007/s11669-021-00871-3

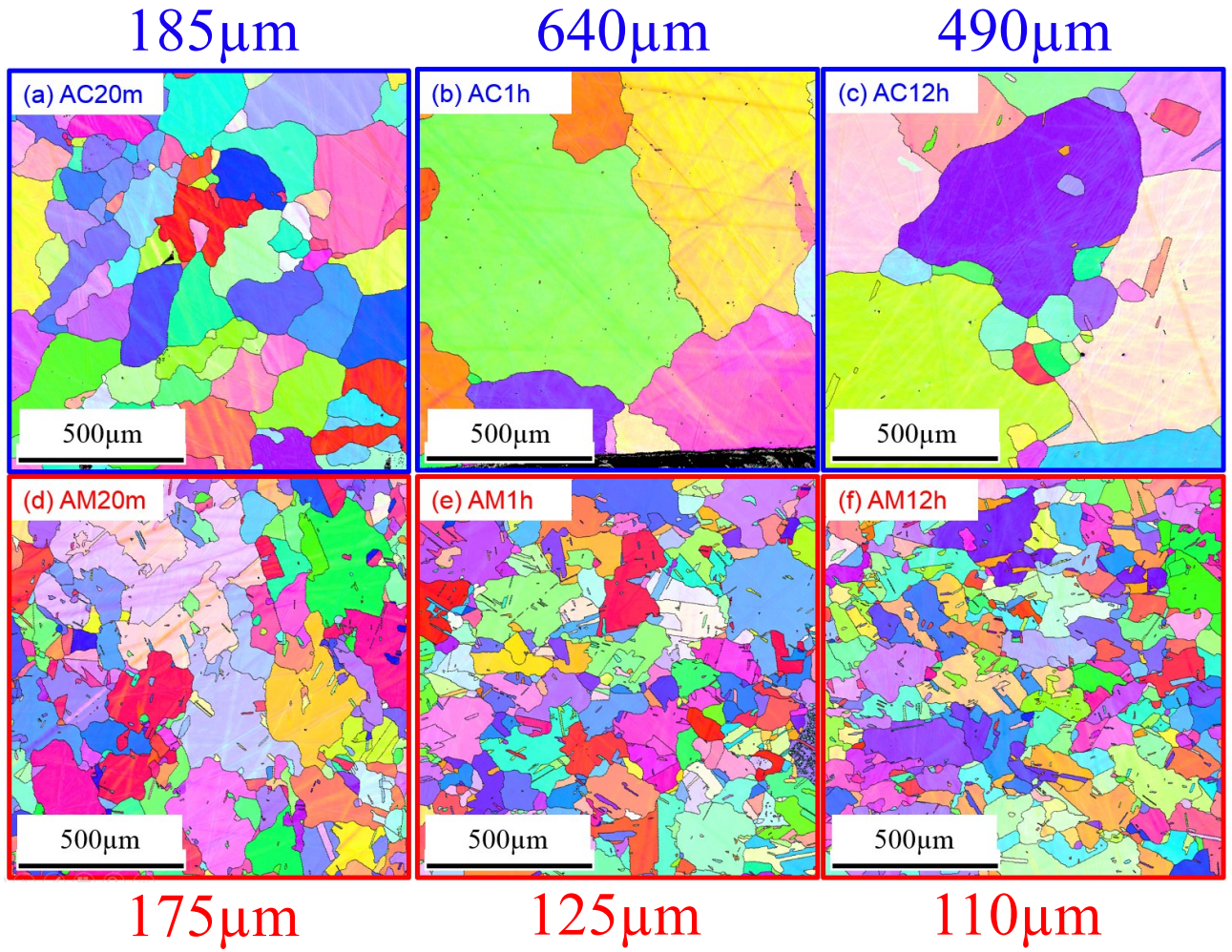
Homogenization of cast and AM samples at 1180°C

- MC, M = Nb as the major element
- MC carbides in cast samples forms in the grains, but MC in AM samples are alone grain boundaries
- The Nb homogeneity are influenced by MC carbide, and thus show inverse tendency in cast and AM samples

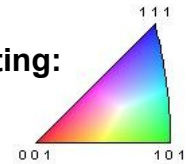


Homogenization of cast and AM samples at 1180°C



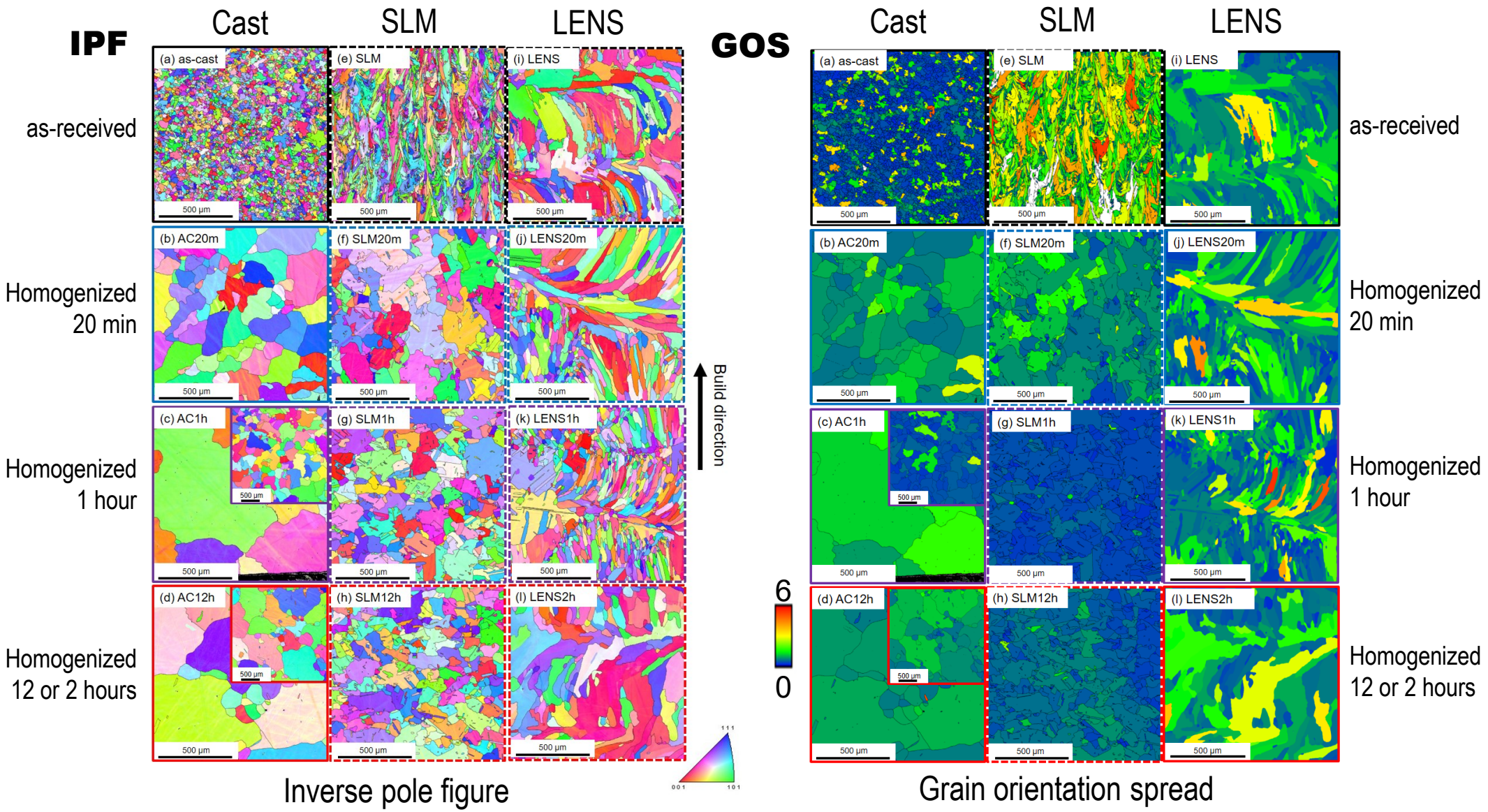


Yunhao Zhao, Kun Li, Matthew Gargani, Wei Xiong, **"A Comparative Analysis of Inconel 718 Made by Additive Manufacturing and Suction Casting: Microstructure Evolution in Homogenization,"** ***Additive Manufacturing***, 36 (2020) 101404. DOI: 10.1016/j.addma.2020.101404



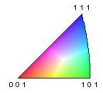
IN718 by LPBF after homogenization at 1180 °C

Noah Sargent, Yuankang Wang, Daozheng Li, Yunhao Zhao, Xin Wang, Wei Xiong, **"Exploring Alloy Design Pathway Through Directed Energy Deposition of Powder Mixtures: A Study of Stainless Steel 316L and Inconel 718,"** ***Additive Manufacturing Letters***, 6 (2023) 100133. DOI: 10.1016/j.addlet.2023.100133

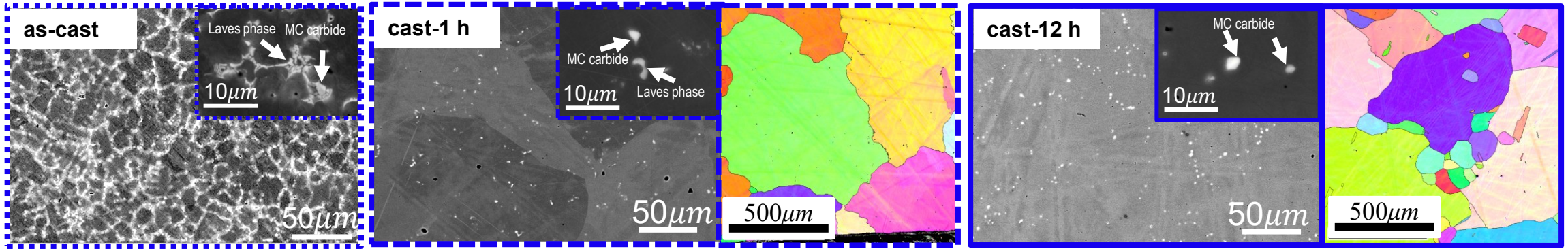


Microstructure of homogenized samples: cast vs. AM

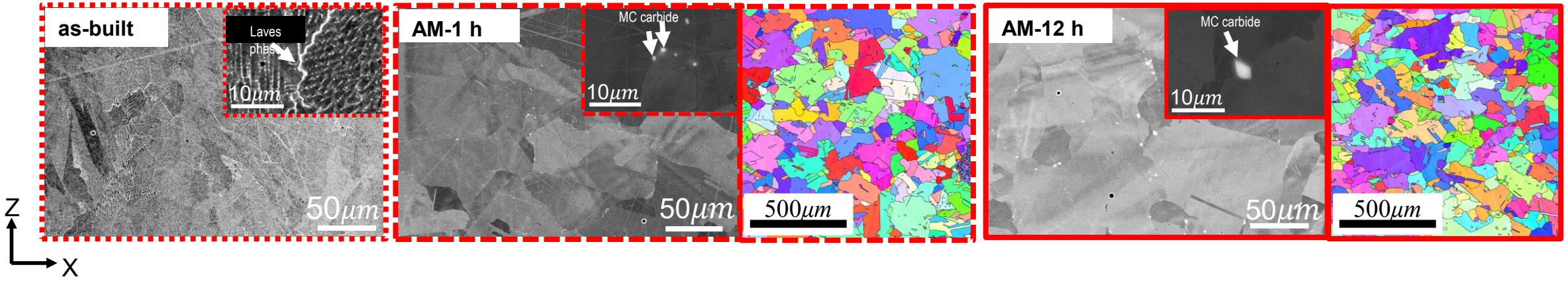
Yunhao Zhao, Fan Meng, Chuan Liu, Susheng Tan, Wei Xiong, **"Impact of homogenization on microstructure-property relationships of Inconel 718 alloy prepared by laser powder bed fusion,"** ***Materials Science and Engineering: A***, 826 (2021) 141973. DOI: 10.1016/j.msea.2021.141973



Cast



AM



Nb homogeneity analysis in the γ matrix close to MC carbide

Nb homogeneity in samples after homogenization at 1180°C

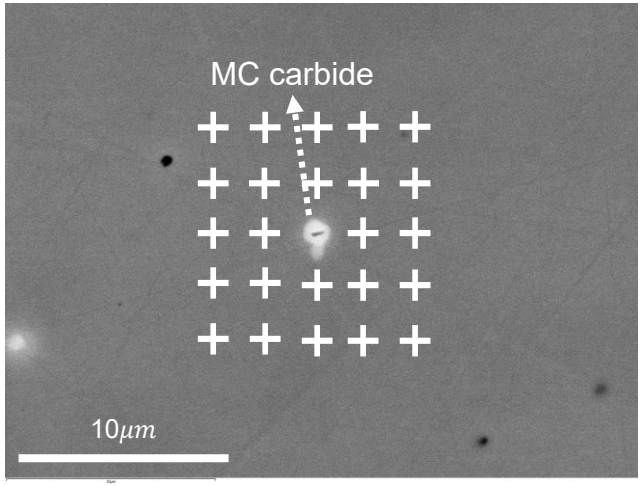
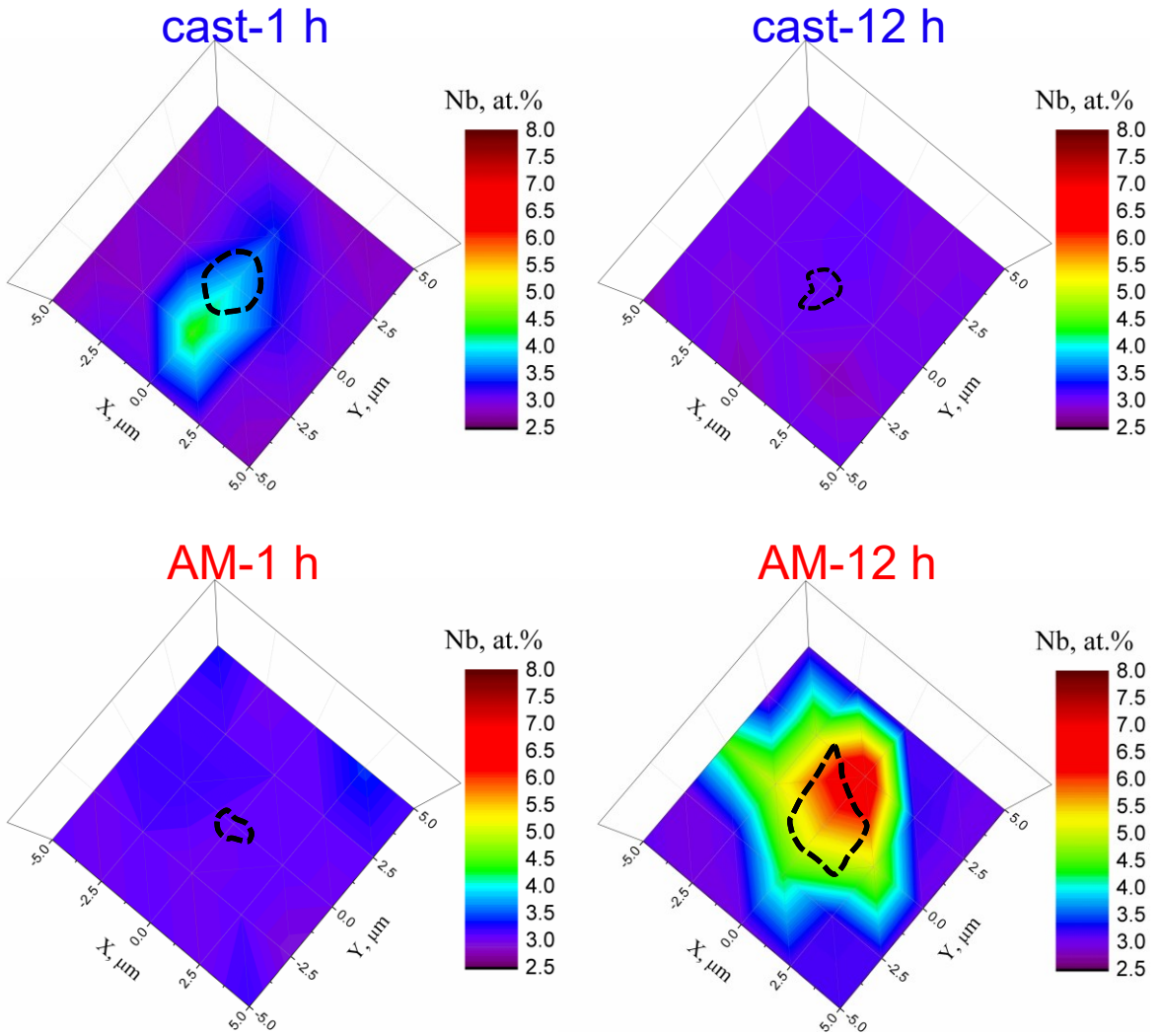


Illustration of Nb concentration EDS mapping



Nb concentration contour diagrams from EDS mapping

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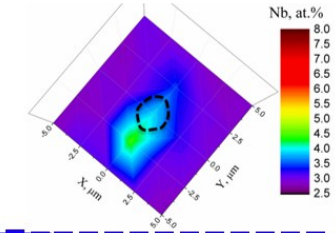
Nb homogeneity analysis in the γ matrix close to MC carbide

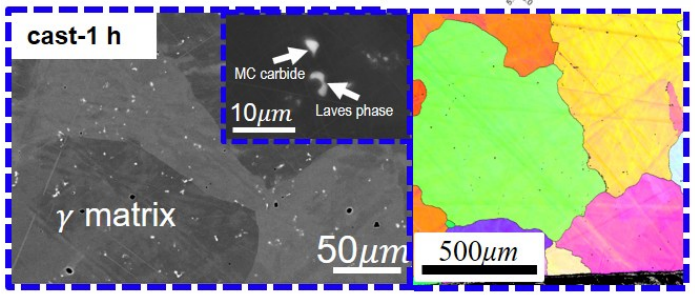
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Nb homogeneity in matrix fcc is bad

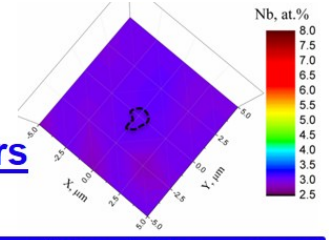


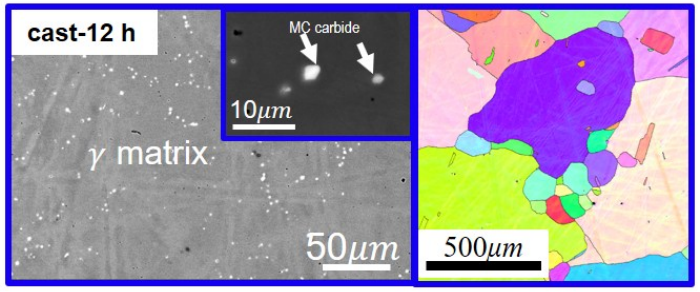
Cast sample Homogenized at 1180°C for **1 hour**





Cast sample Homogenized at 1180°C for **12 hours**





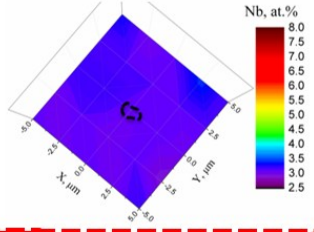
Nb homogeneity in matrix fcc is good

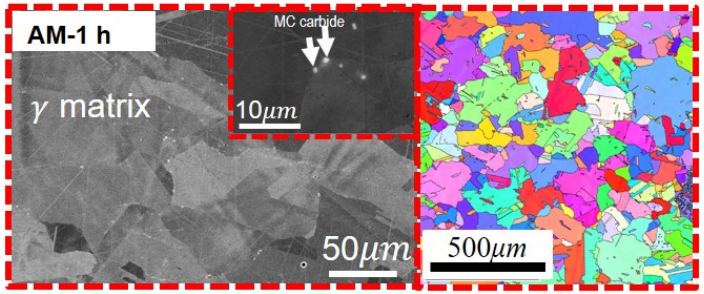


Nb homogeneity in matrix fcc is good

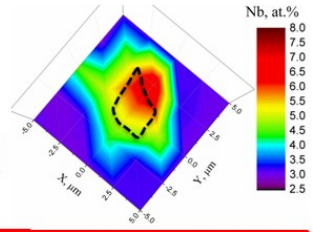


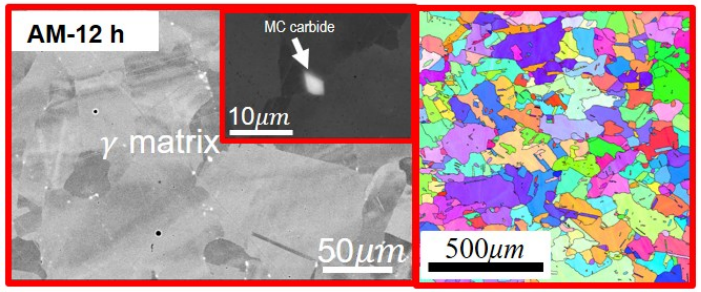
AM sample Homogenized at 1180°C for **1 hour**





AM sample Homogenized at 1180°C for **12 hours**





Nb homogeneity in matrix fcc is bad

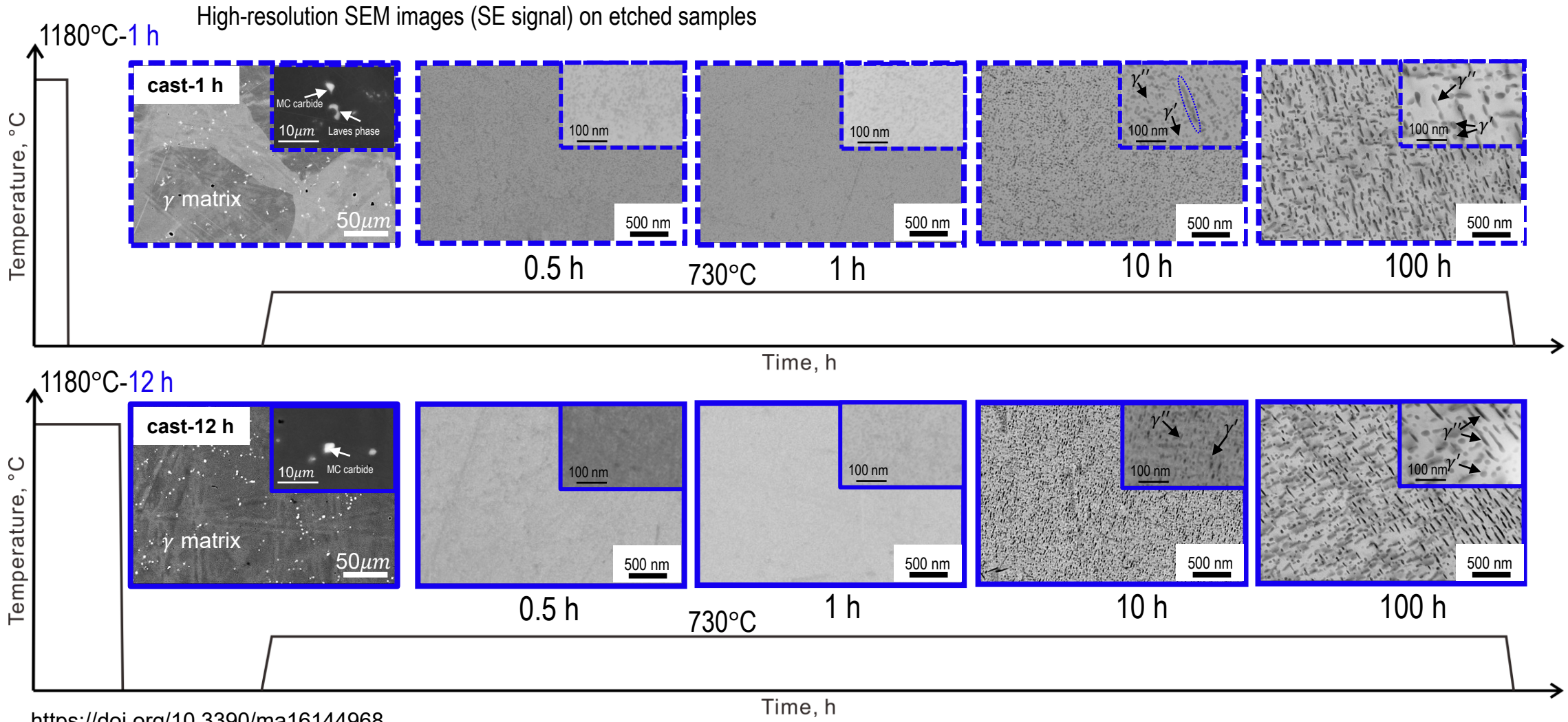


- Effects of **homogenization time** on phase transformation kinetics at 730°C
- Effects of **manufacturing methods** on phase transformation kinetics at 730°C

Zhao, Y.; Xiong, W. Influence of Homogenization on Phase Transformations during Isothermal Aging of Inconel 718 Superalloys Fabricated by Additive Manufacturing and Suction Casting. *Materials* **2023**, *16*, 4968. https://doi.org/10.3390/ma16144968

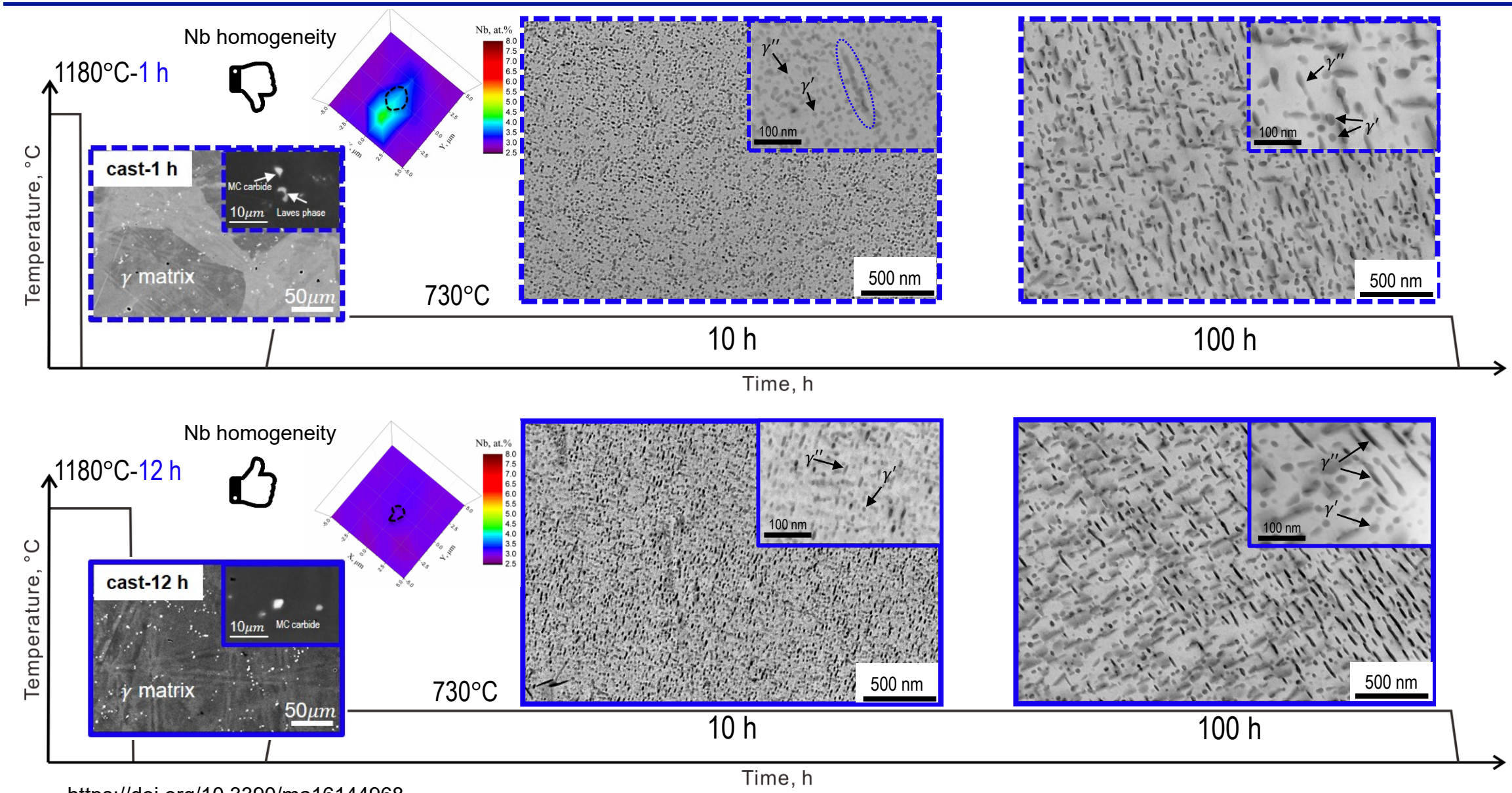
Homogenization influence on precipitation at 730°C: Cast Samples

γ''/γ' precipitation starts to form at about 10 h at 730°C under both homogenization conditions.



https://doi.org/10.3390/ma16144968

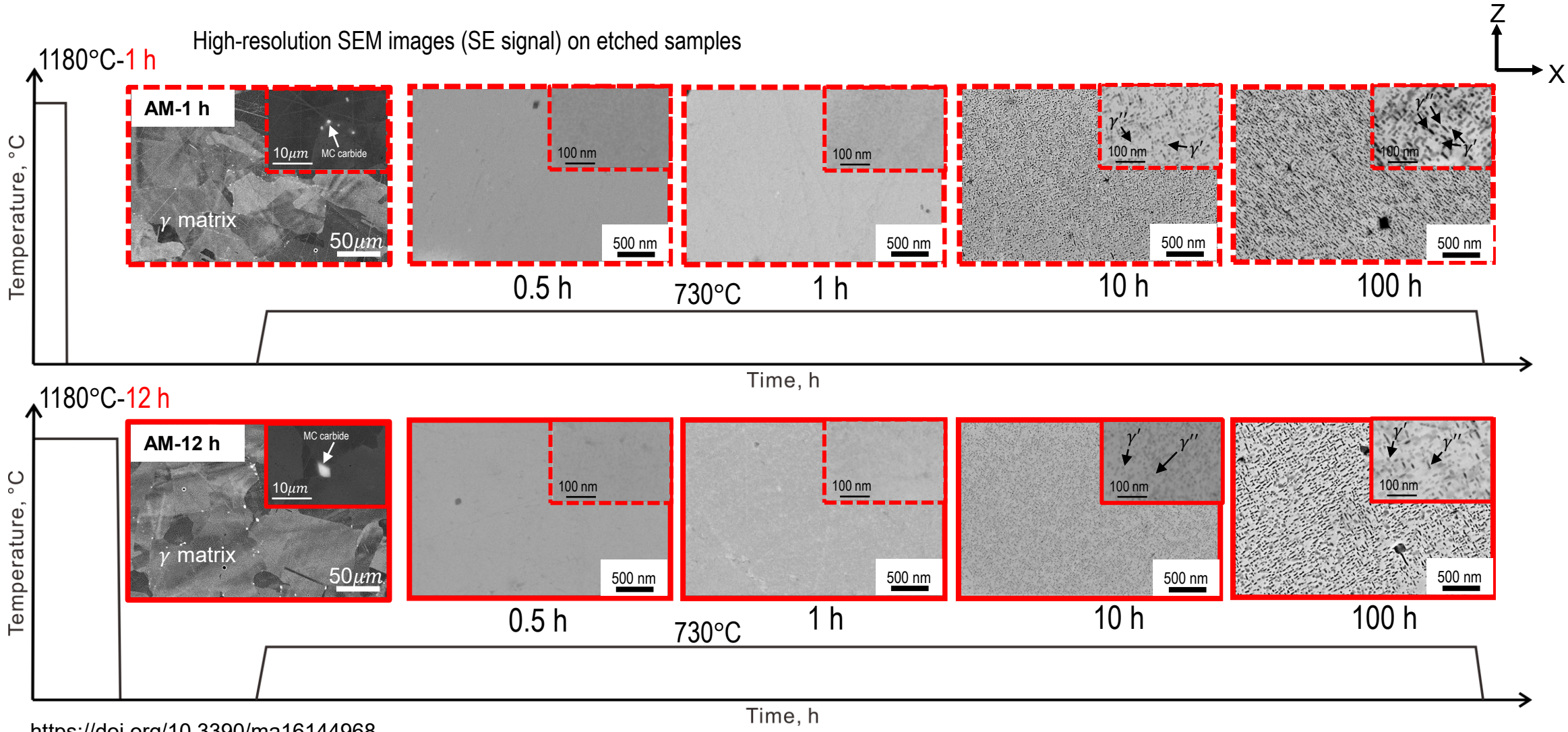
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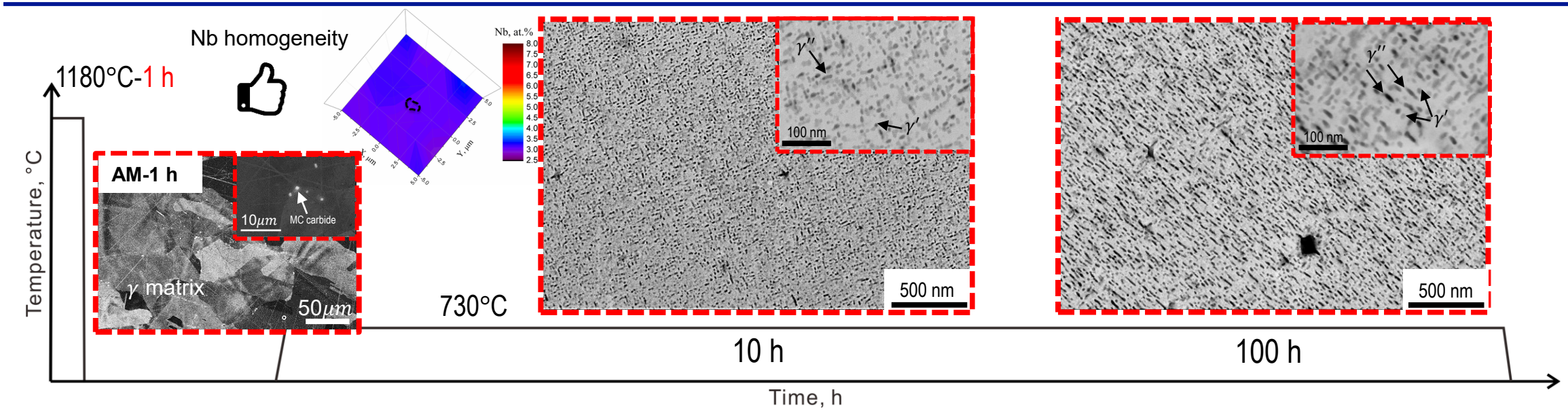
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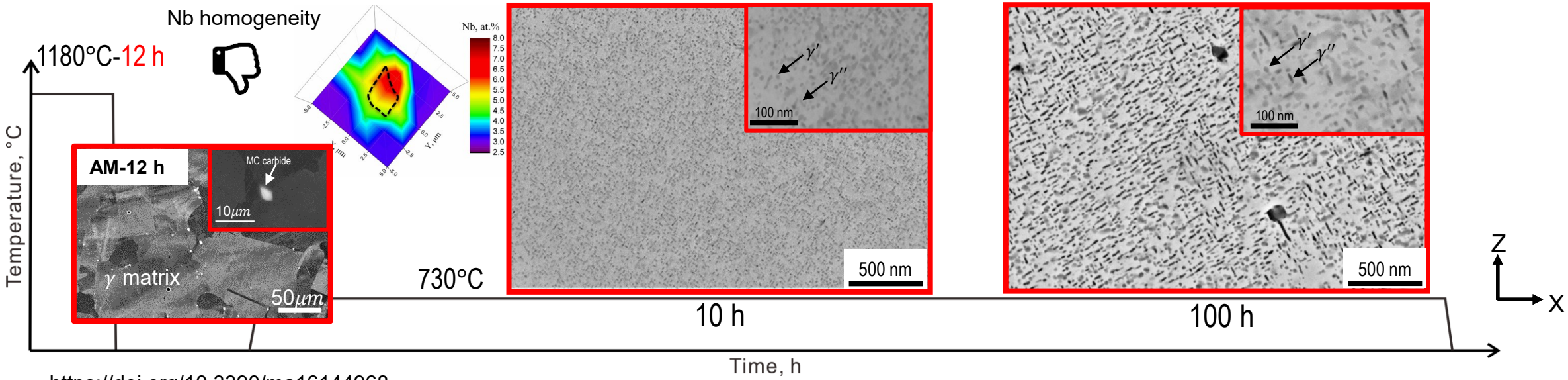
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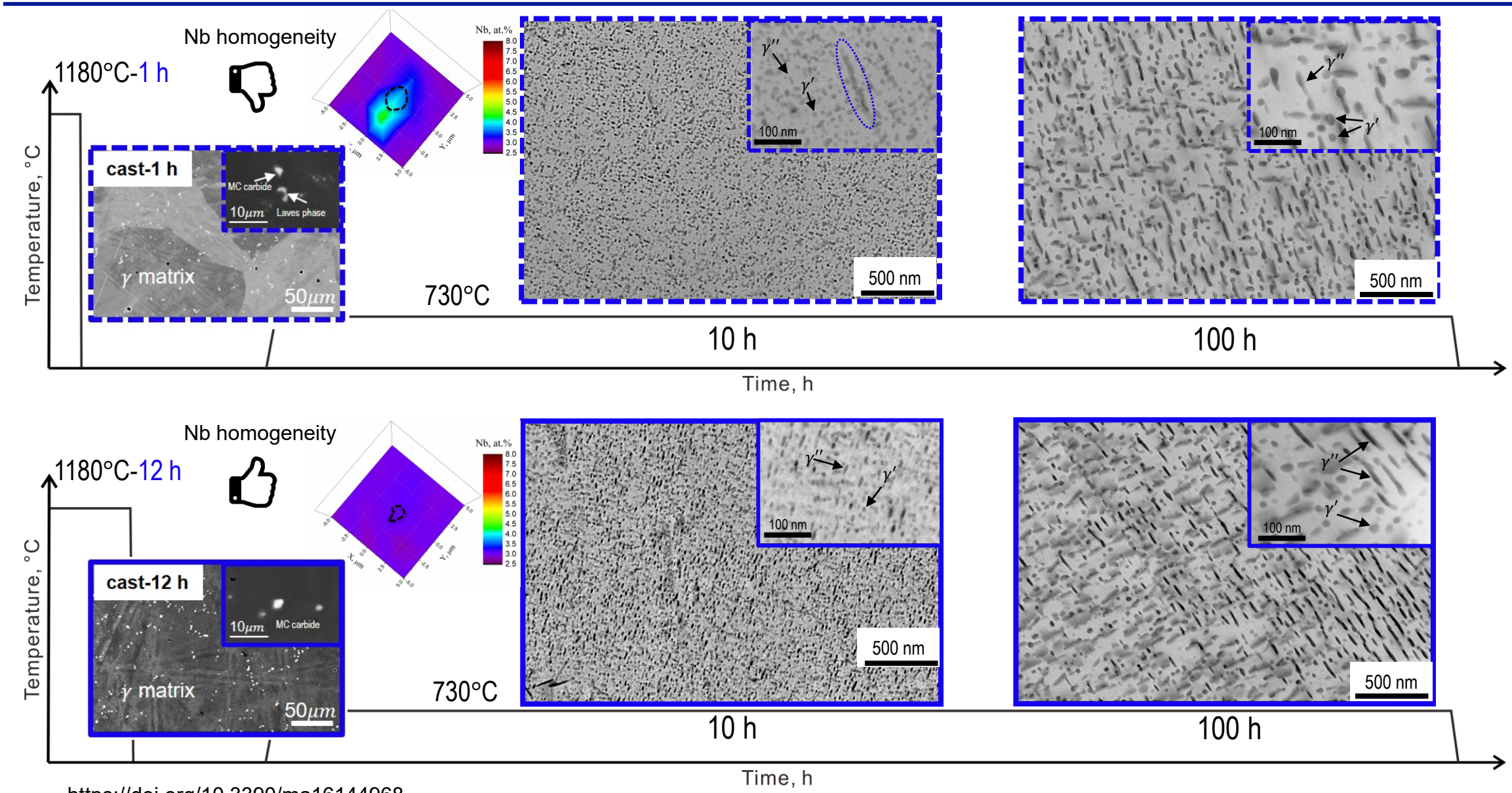
Homogenization influence on precipitation at 730°C: AM samples





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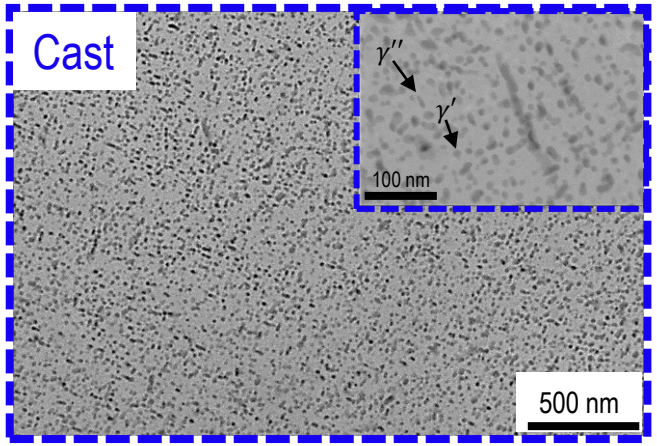


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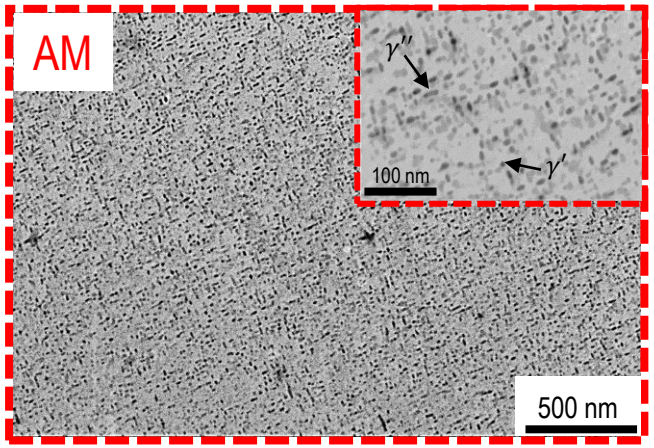
Effects of manufacturing methods: cast & AM samples

1180°C, 1h ➔ 730°C, 10h

Nb homogeneity

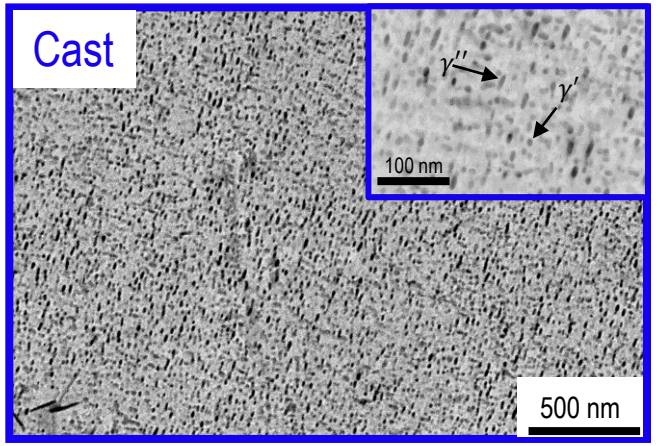


Nb homogeneity

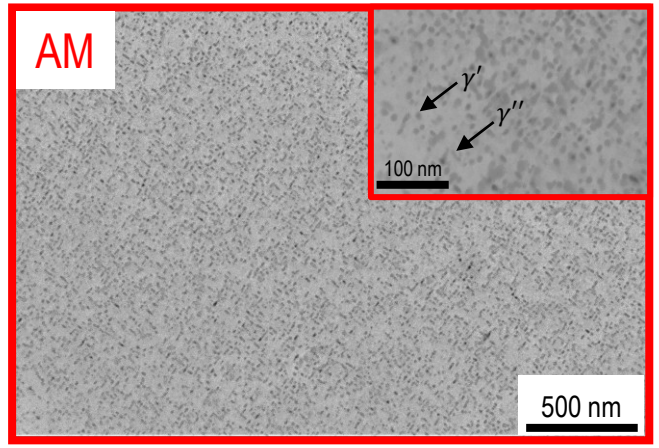


1180°C, 12h ➔ 730°C, 10h

Nb homogeneity

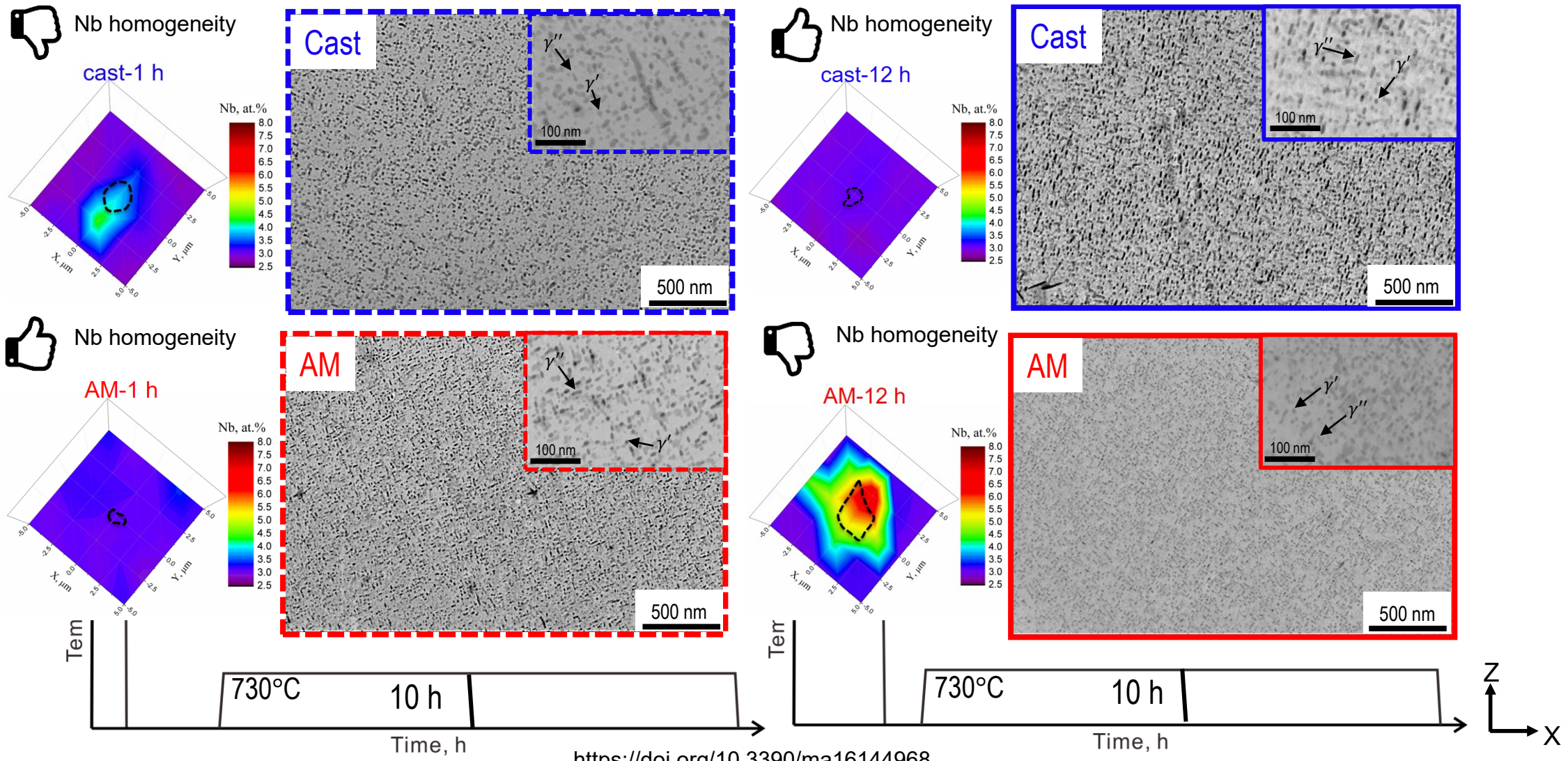


Nb homogeneity



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Effects of manufacturing methods: cast & AM samples (730°C, 10h)

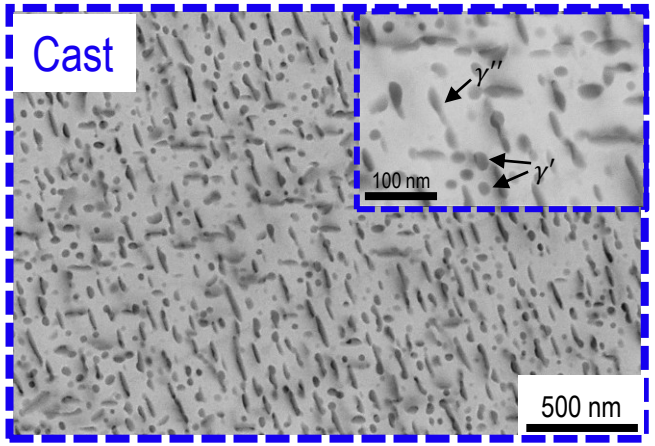


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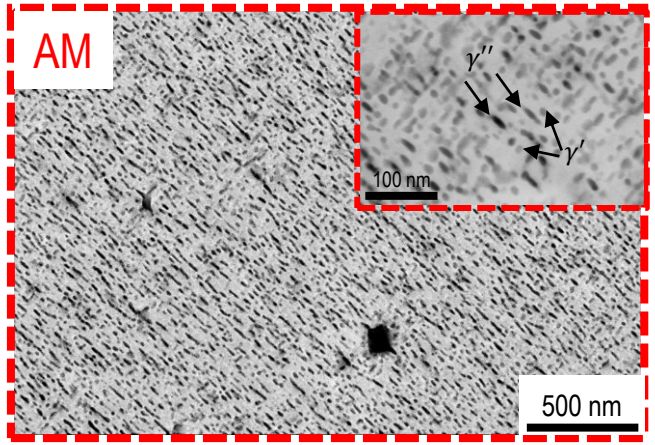
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Nb homogeneity

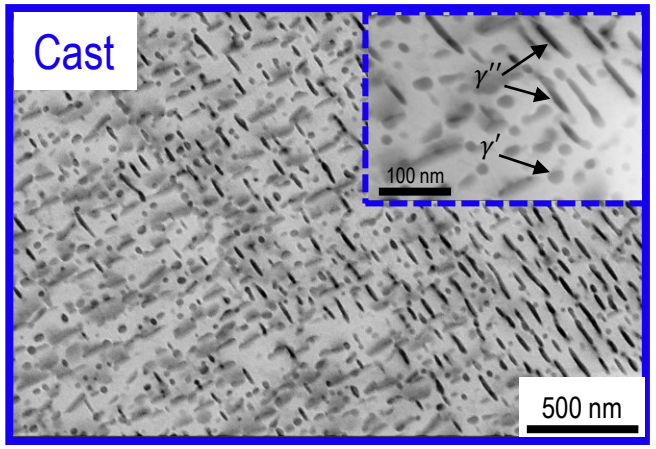


Nb homogeneity

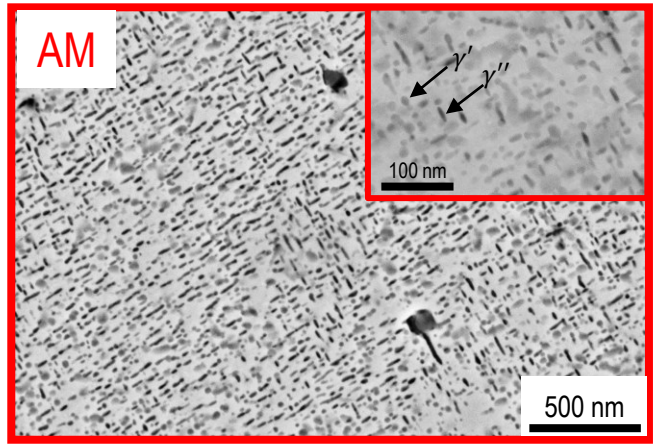


1180°C, 12h ➔ 730°C, 100h

Nb homogeneity

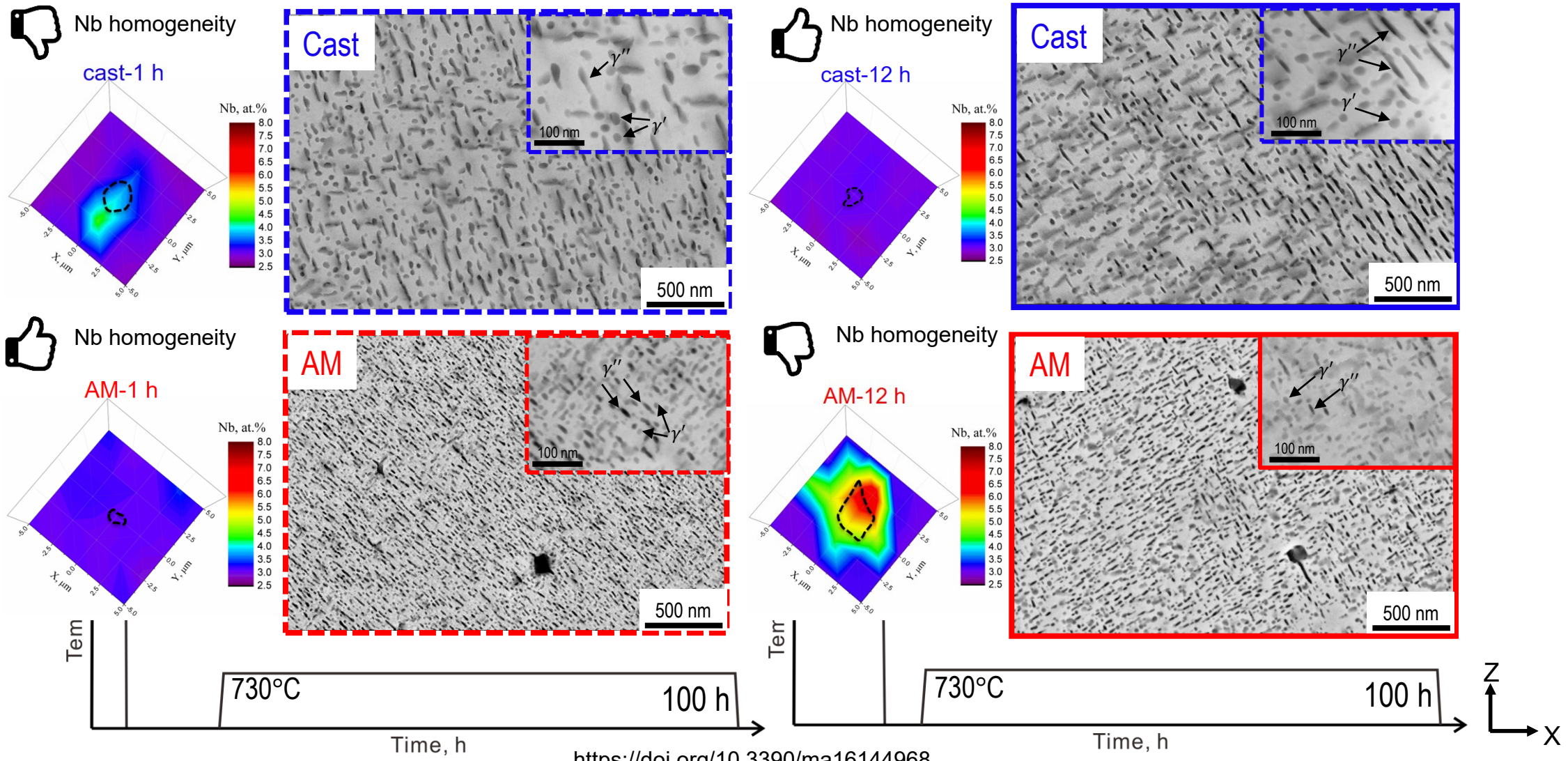


Nb homogeneity



https://doi.org/10.3390/ma16144968

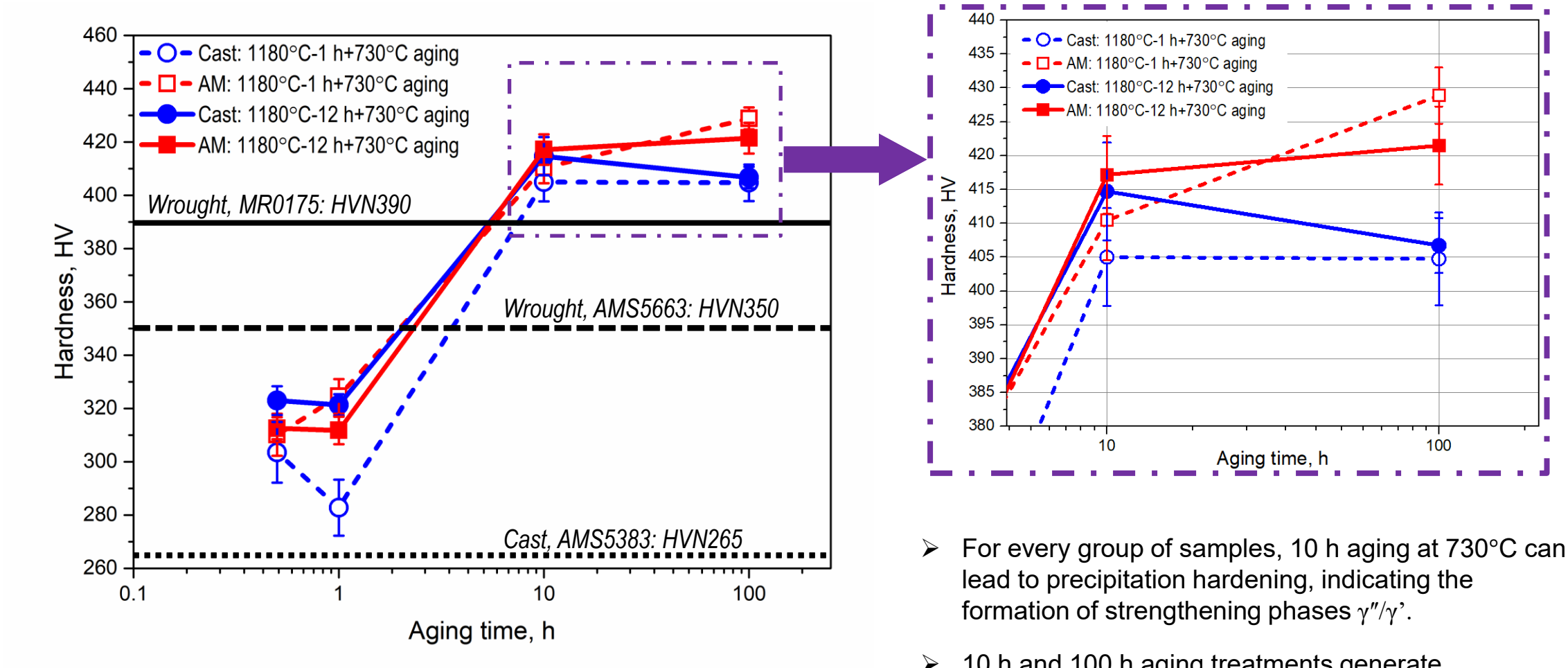
Effects of manufacturing methods: cast & AM samples (730°C, 100h)



https://doi.org/10.3390/ma16144968

Hardness tests: Cast vs. AM

Zhao, Y.; Xiong, W. Influence of Homogenization on Phase Transformations during Isothermal Aging of Inconel 718 Superalloys Fabricated by Additive Manufacturing and Suction Casting. *Materials* **2023**, *16*, 4968. https://doi.org/10.3390/ma16144968



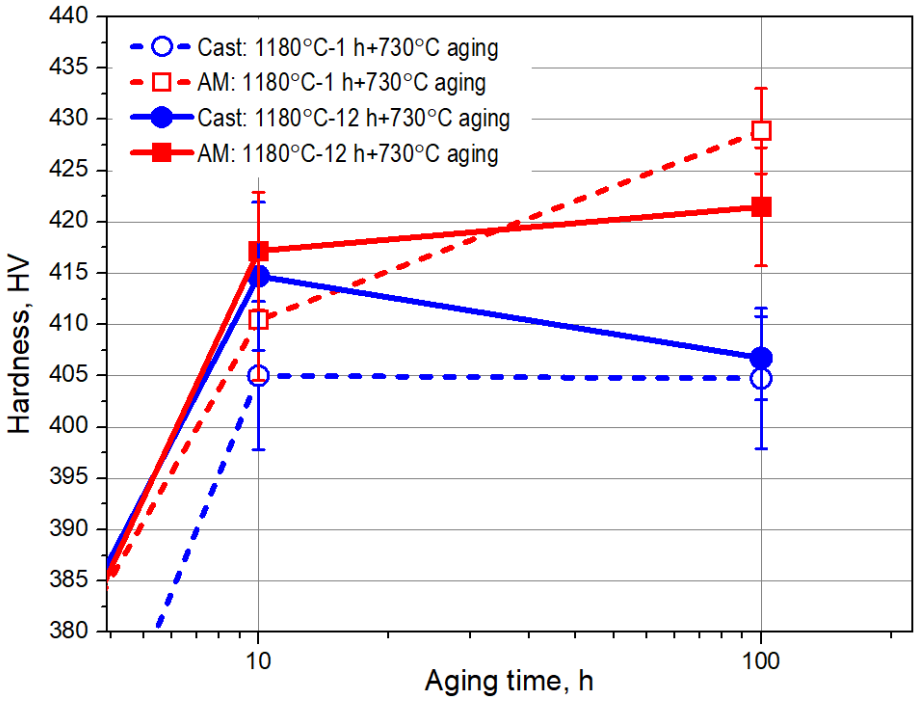
Vickers hardness testing results on aged samples
(AM samples are tested on XZ plane)

- For every group of samples, 10 h aging at 730°C can lead to precipitation hardening, indicating the formation of strengthening phases γ″/γ’.
- 10 h and 100 h aging treatments generate comparable hardness in all group of samples.
- After 10 h aging, the hardness of AM samples starts to exceed that of AC samples.

D. Zhang, W. Niu, X. Cao, Z. Liu, Mater. Sci. Eng. A 64 (2015) 32–40

https://www.aircraftmaterials.com/data/nickel/718.html

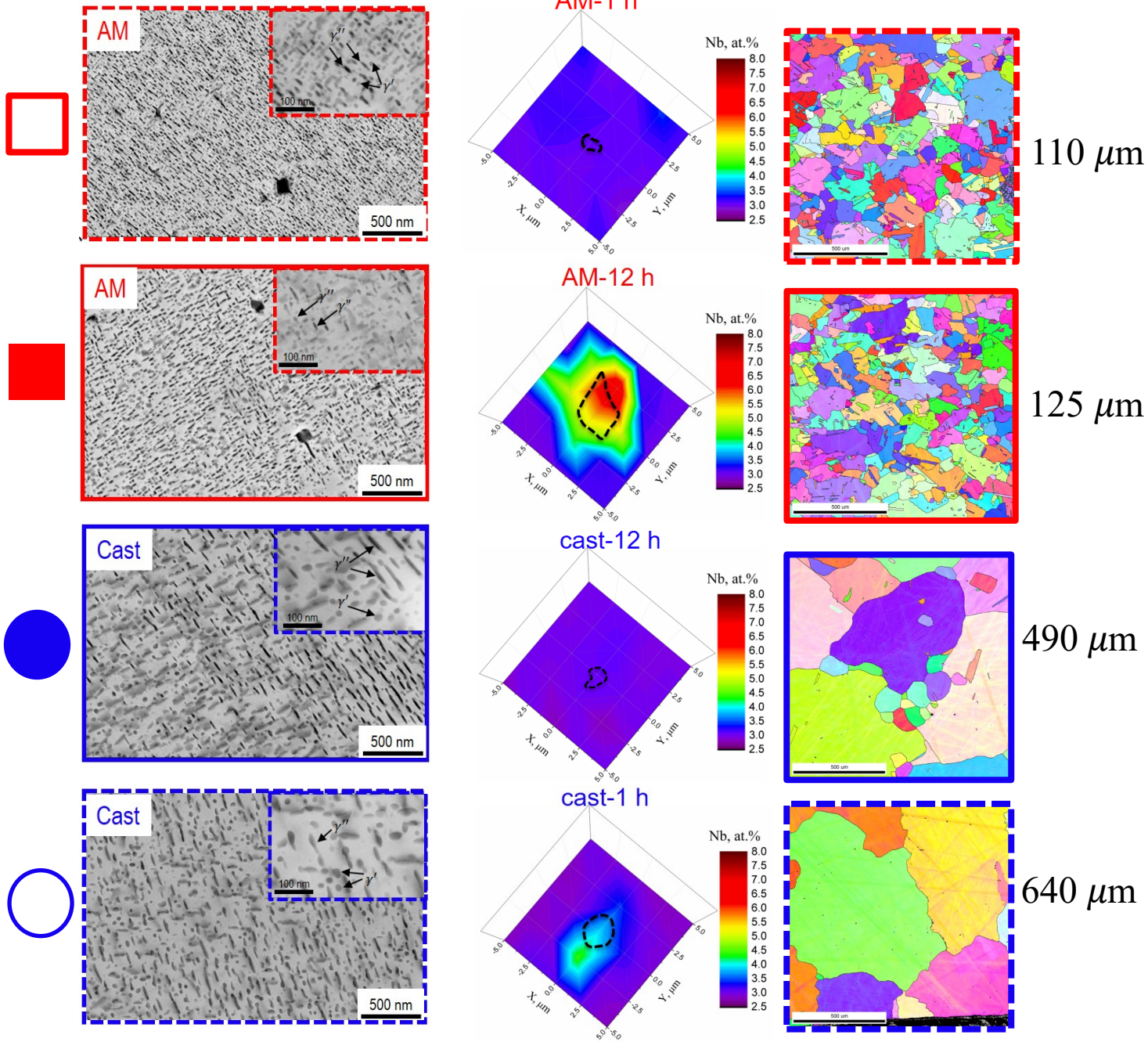
http://www.specialmetals.com/assets/smc/documents/inconel_alloy_718.pdf



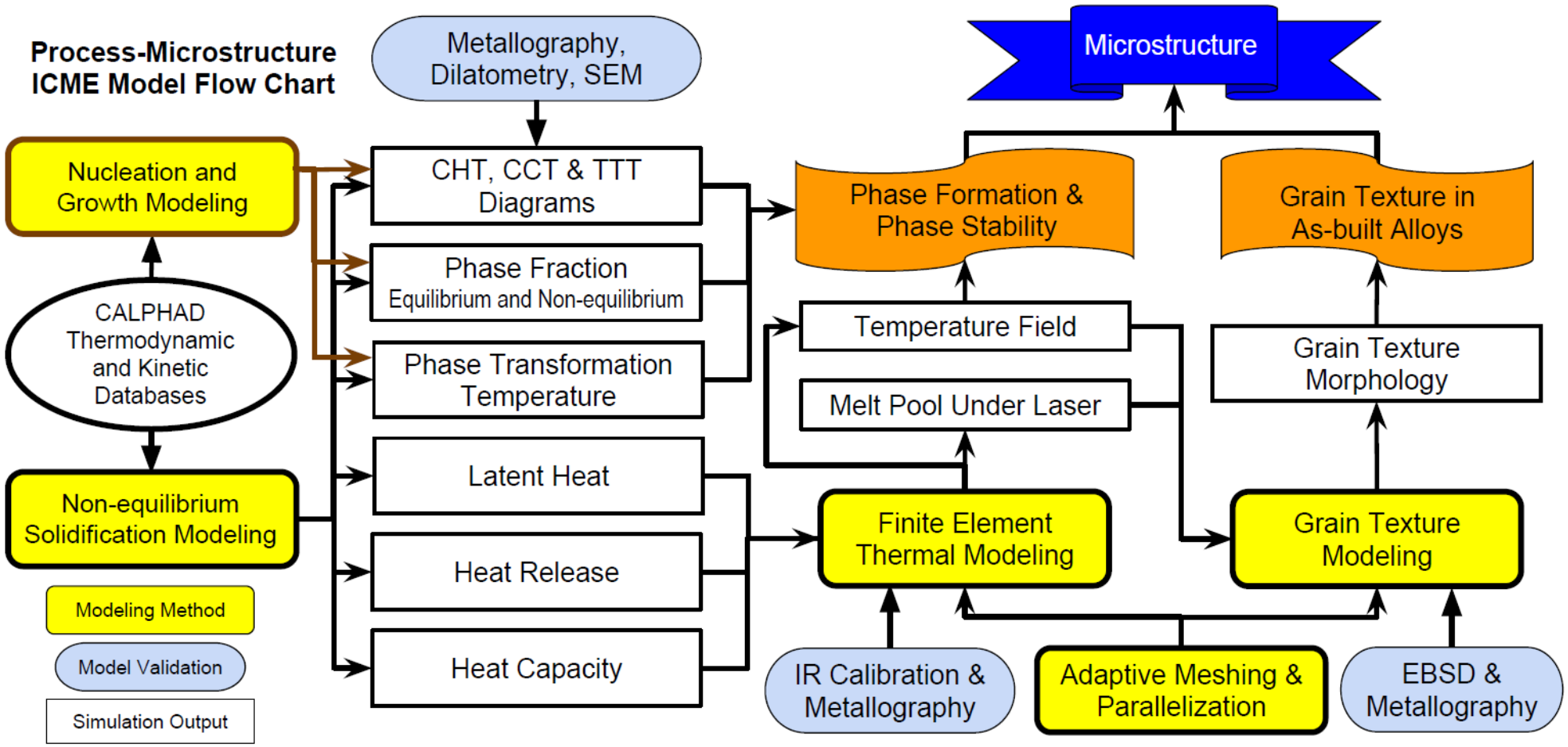
Homogenization can influence the phase distribution and fraction in both cast and AM alloys.

In AM alloys, homogenization can influence the mechanical performance

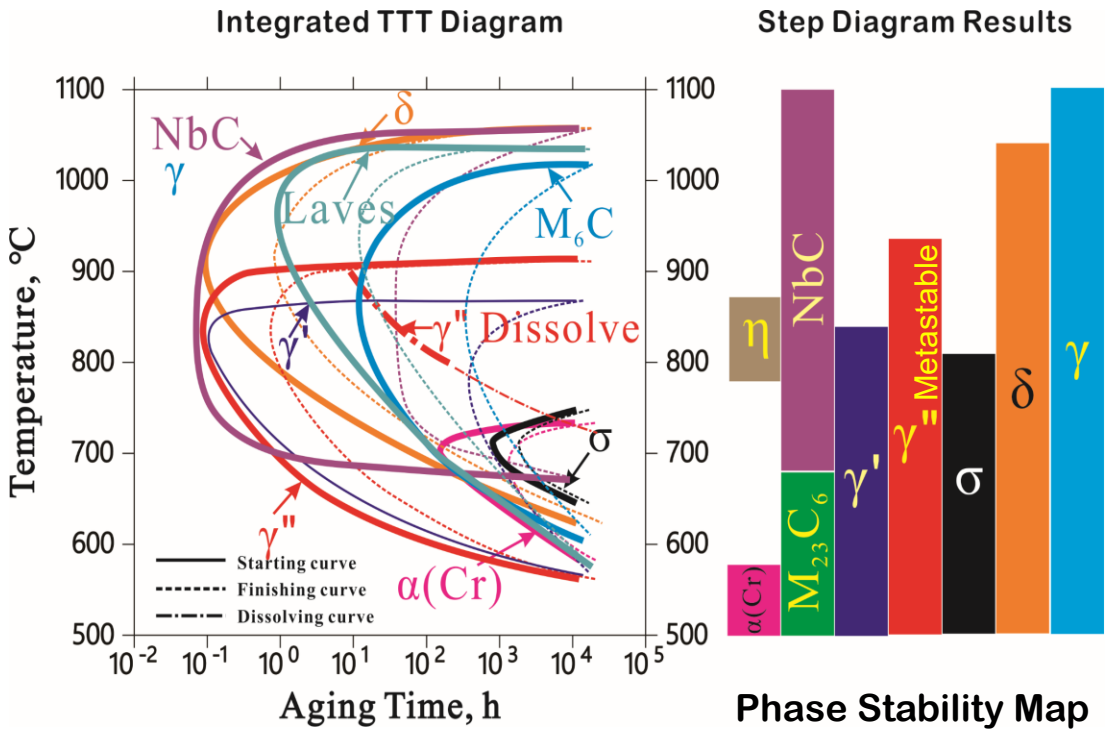
730°C, 100h ⇦ 1180°C, 1h or 12h

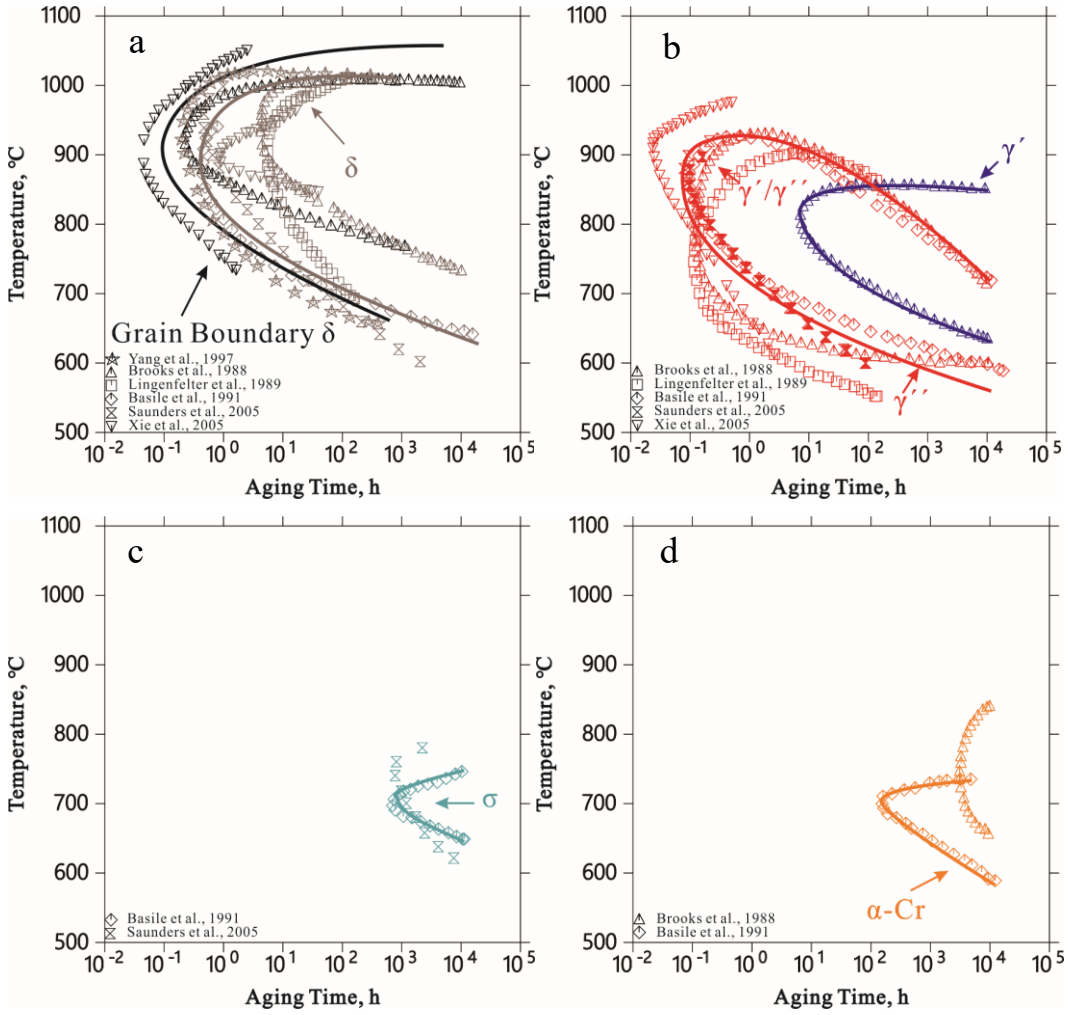


CALPHAD method for laser powder bed simulation



TTT (Temperature-Time-Transformation) Diagram of Inconel 718

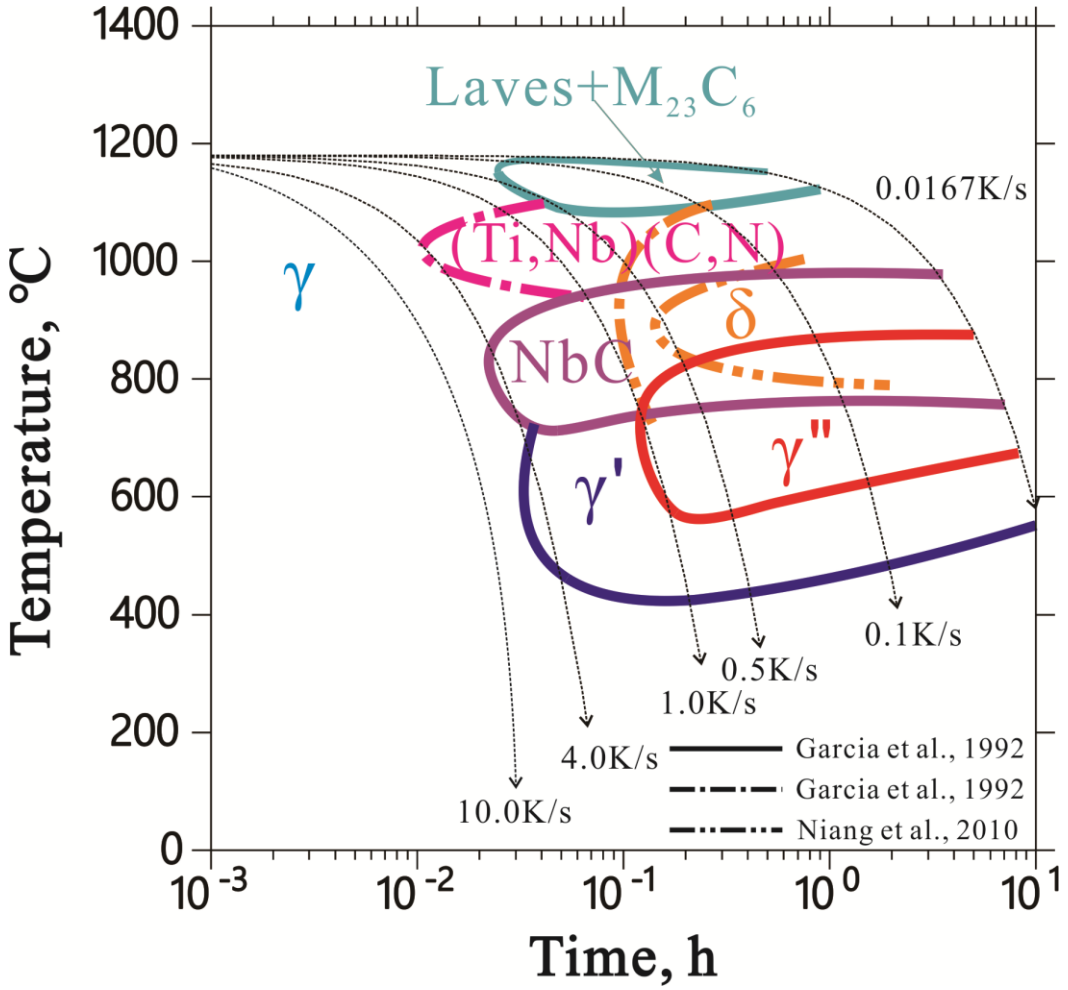




Yunhao Zhao, Liangyan Hao, Qiaofu Zhang, Wei Xiong, Phase transformations during continuous cooling in Inconel 718 alloys manufactured by laser powder bed fusion and suction casting, Materials Characterization, 185 (2022) 111764, https://doi.org/10.1016/j.matchar.2022.111764.

[1988Bro] Brooks J, Bridges P. Metallurgical stability of inconel alloy 718. Superalloys 1988;88:33-42.
[1989Lin] Lingenfelter A. Welding of Inconel alloy 718: A historical overview. Superalloy 1989;718:673-83.
[1991Ora] Oradei-Basile A, Radavich JF. A current TTT diagram for wrought alloy 718. Superalloys 1991;718:325-35.
[2005Xie] Xie X, Xu C, Wang G, Dong J, Cao W-D, Kennedy R. Sixth International Special Emphasis Symposium on Superalloys 718, 625, 706 and Derivatives2005. p. 193-202.

CCT (Continuous-Cooling-Transformation) Diagram of Inconel 718



NB: Disregarding grain size impact, there are still debates about phase transformation information of Inconel 718 shown in CCT/TTT diagrams!

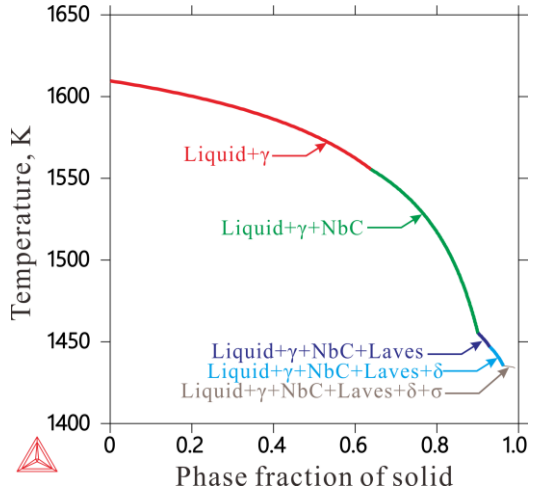
- Slama [1997Sla] et al. determined a curve for the $\gamma' + \gamma''$ two phase region, which deviates a lot from that by Garcia et al. [1992Gar], due to short homogenization time of the samples used in their work.
- Niang et al. [2010Nia] got the CCT of δ phase, but also has a big difference with that of Garcia et al. [1992Gar]

Yunhao Zhao, Liangyan Hao, Qiaofu Zhang, Wei Xiong, Phase transformations during continuous cooling in Inconel 718 alloys manufactured by laser powder bed fusion and suction casting, Materials Characterization, 185 (2022) 111764, https://doi.org/10.1016/j.matchar.2022.111764.

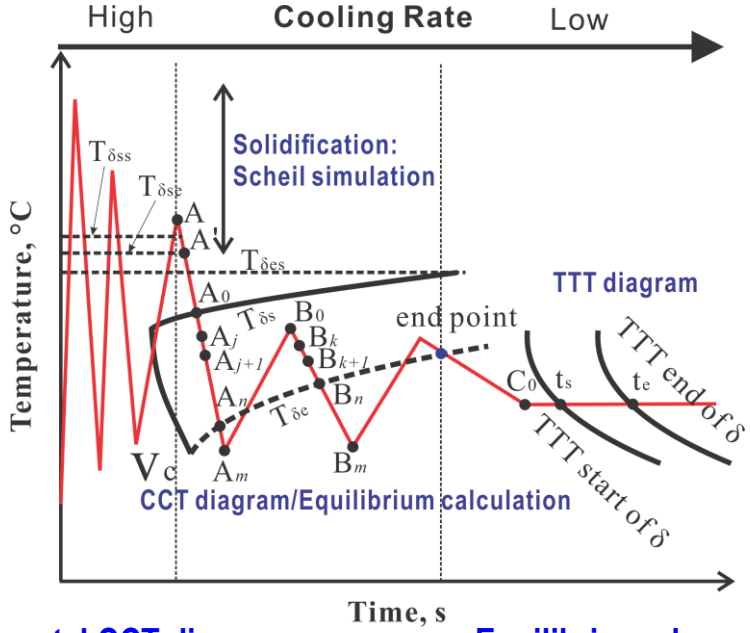
[1992Gar] Garcia C, Lis A, Loria E, DeArdo A. Thermomechanical Processing and Continuous Cooling Transformation Behavior of IN 718. Proc Conf Superalloys1992. p. 527-36.
[1997Sla] Slama C, Cizeron G. Étude du comportement structural de l'alliage NC 19 Fe Nb (Inconel 718). Journal de Physique III 1997;7:665-88.
[2010Nia] Niang A, Viguier B, Lacaze J. Some features of anisothermal solid-state transformations in alloy 718. Materials Characterization 2010;61:525-34.

ICME modeling framework: the δ phase

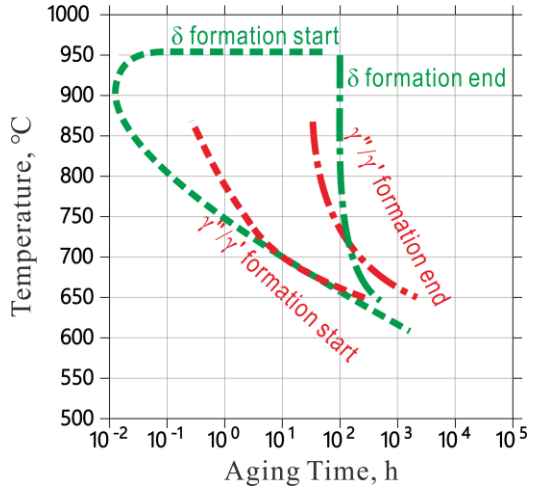
Scheil simulation



1. Solidification modeling

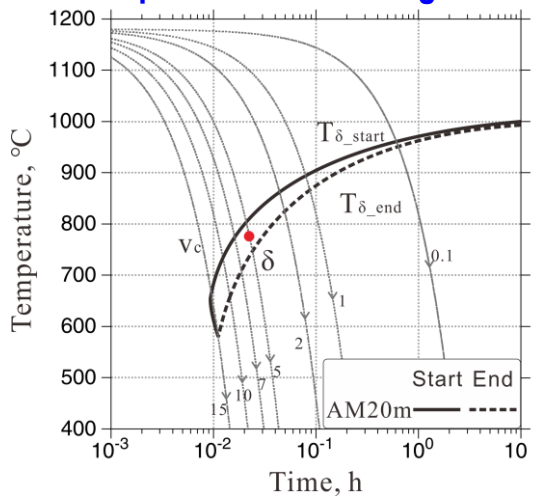


Evaluated TTT diagram



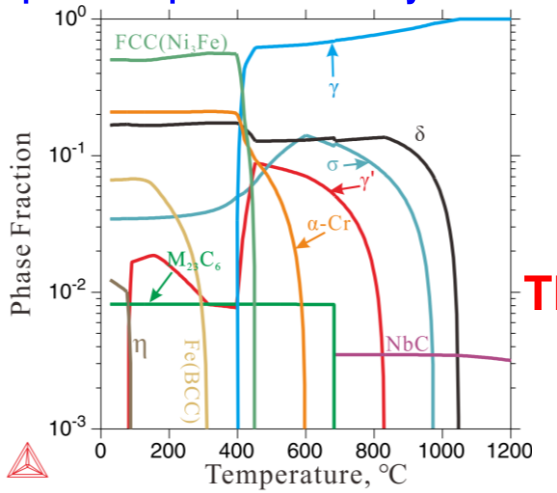
4. Isothermal process modeling

Experimental CCT diagram



2. Cooling process modeling

Equilibrium phase fraction by CALPHAD

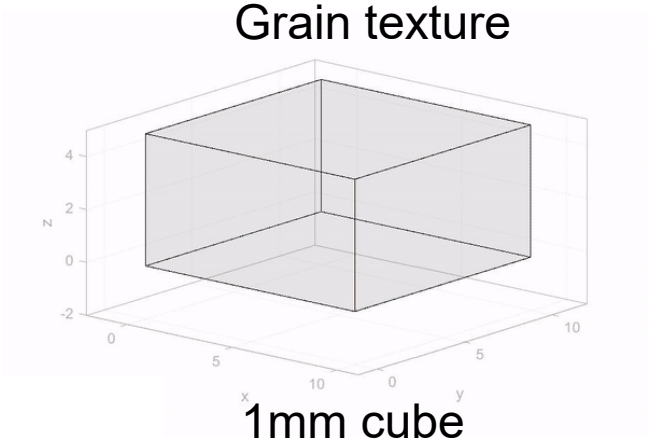


3. Heating process modeling

This is an *approximation*

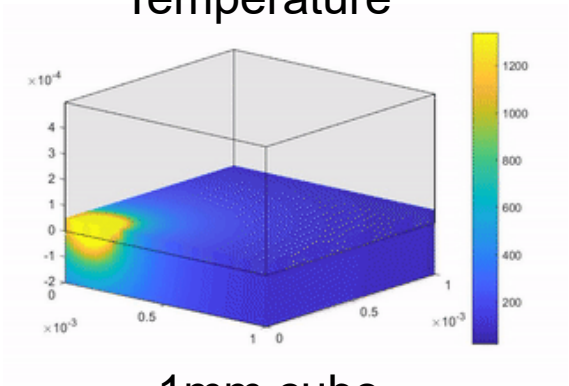
Case study on Inconel 718 superalloy under selected laser melting

Grain texture



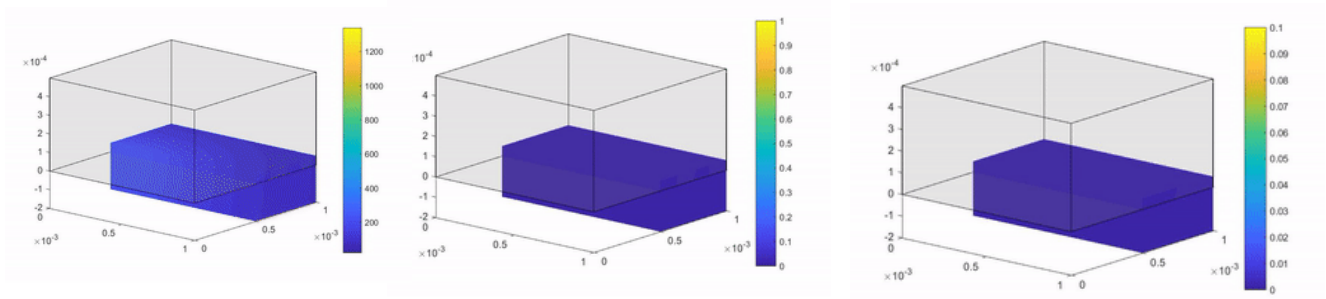
1mm cube

Temperature



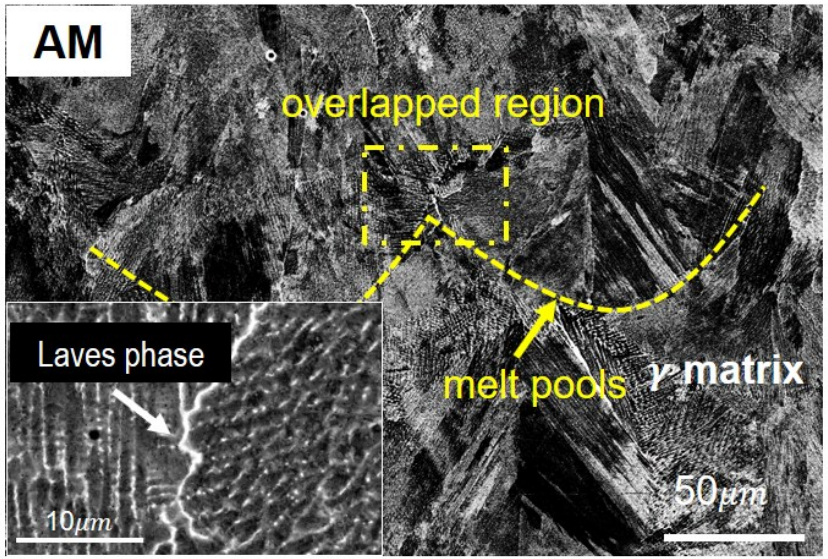
1mm cube

- Simulation of grain growth(texture) and FEM simulation
- Consideration of multi-phase transformation



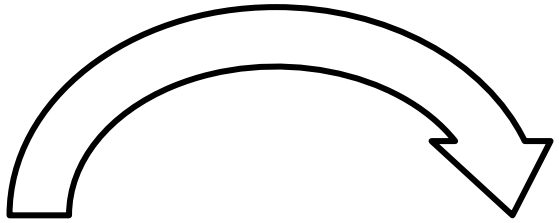
Temperature Liquid fraction Laves/δ fraction

1mm cube



Microstructure of as-built Inconel 718

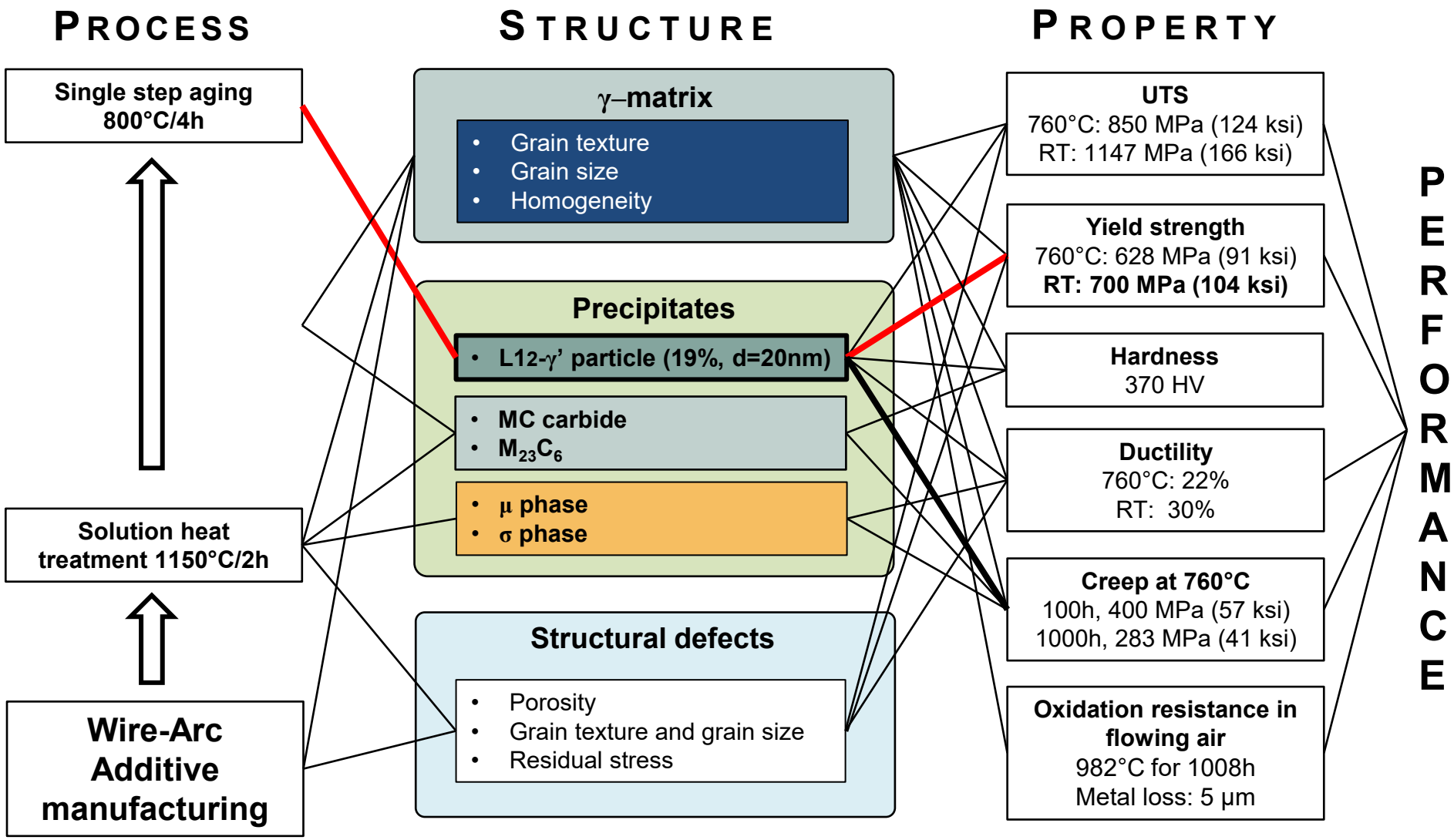
LPBF (laser powder bed fusion) *vs.* WAAM (wire-arc AM)



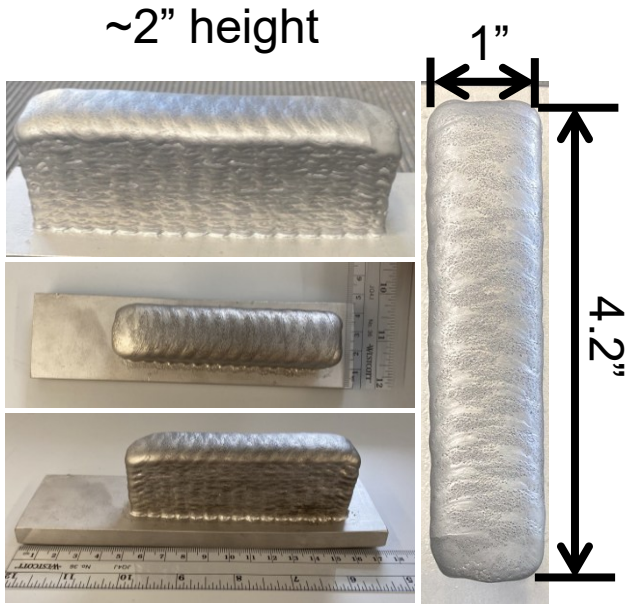
	Case 1	Case 2
Materials	Inconel 718	Haynes 282
Method	LPBF	WAAM

Methodology: Systems design chart for Haynes 282

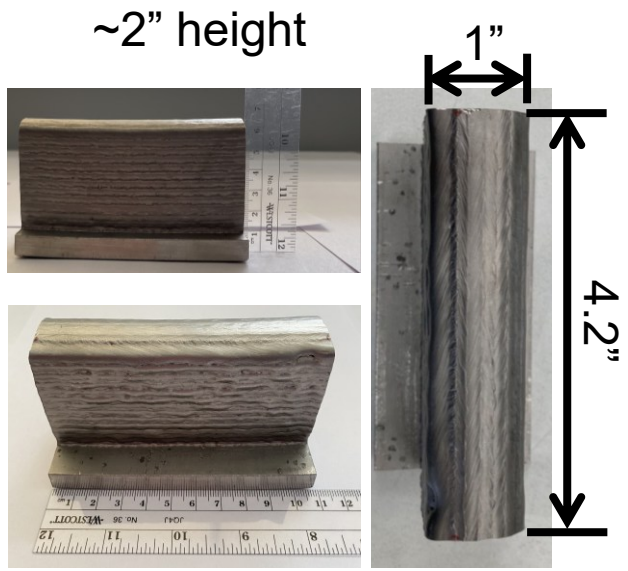
Demonstrates how hierarchical structural features contribute to the properties along with the evolution of the structure during different processing conditions



Haynes 282 Printing strategy difference: Meander vs. Single Bead

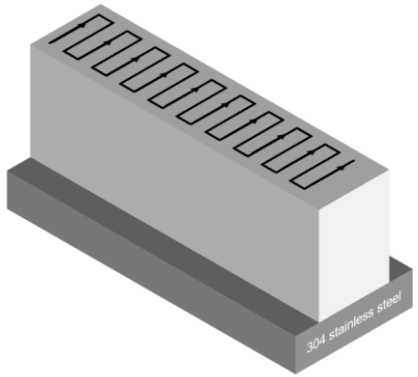


Multitrack Meander Haynes 282

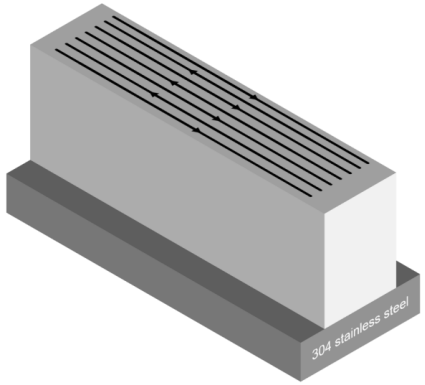


Multitrack Single Bead Haynes 282

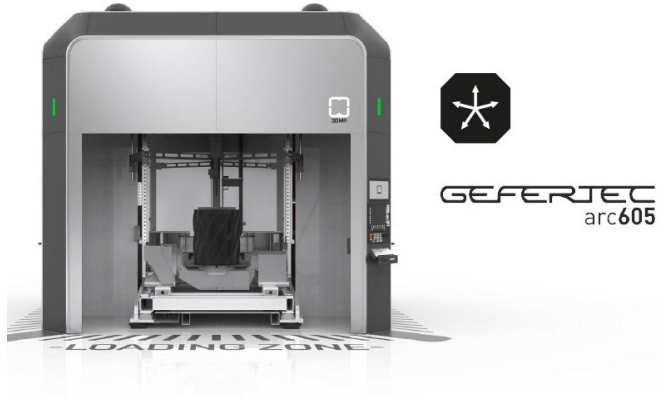
Luis Fernando Ladinos Pizano, Soumya Sridar, Rafael Rodriguez De Vecchis, Xin Wang, Jacob Biddlecom, Garrett J. Pataky, Chantal Sudbrack, Wei Xiong, Journal of Manufacturing Processes, 119 (2024) 781–789, https://doi.org/10.1016/j.jmapro.2024.04.015



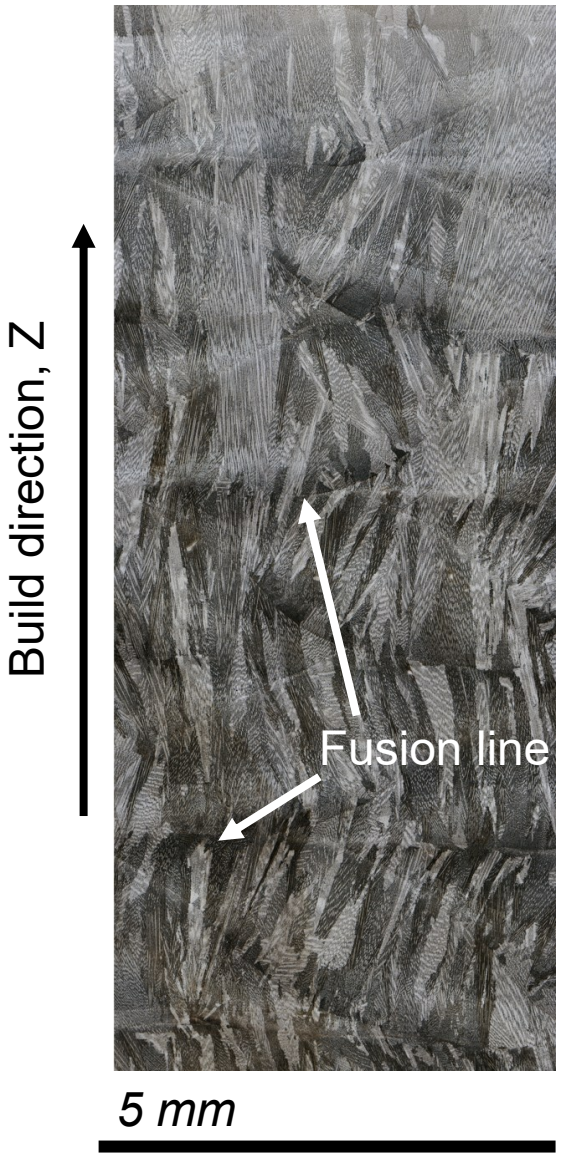
Zigzag, Meander



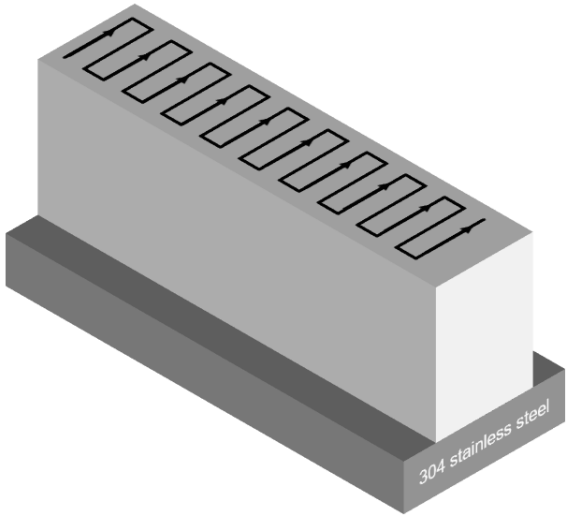
Single bead



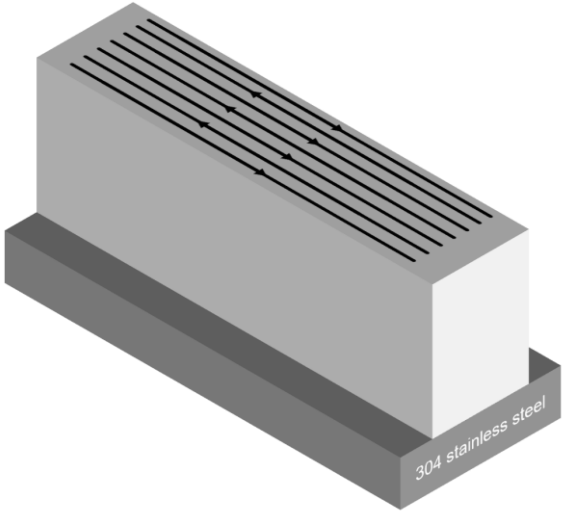
As-printed microstructure: Meander vs. Single Bead



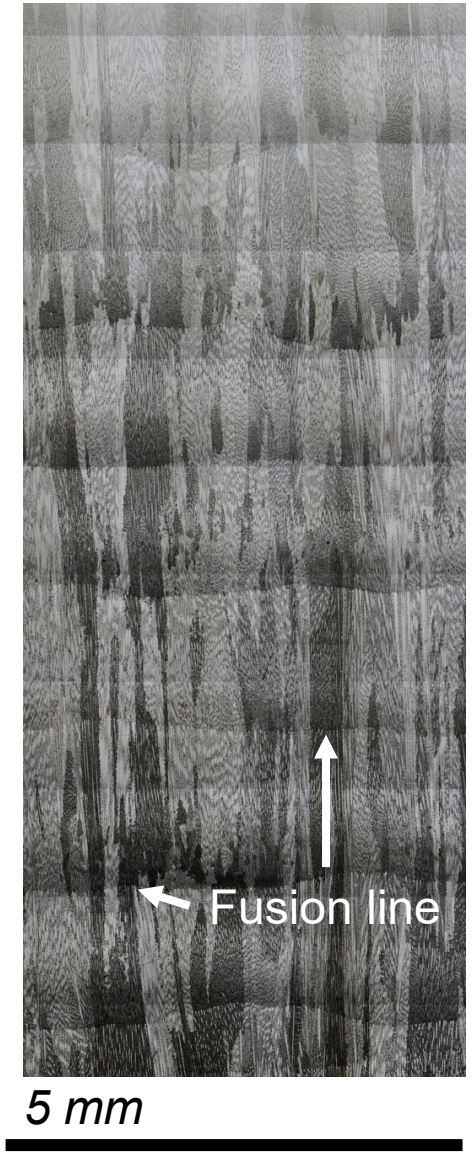
Single bead



vs.

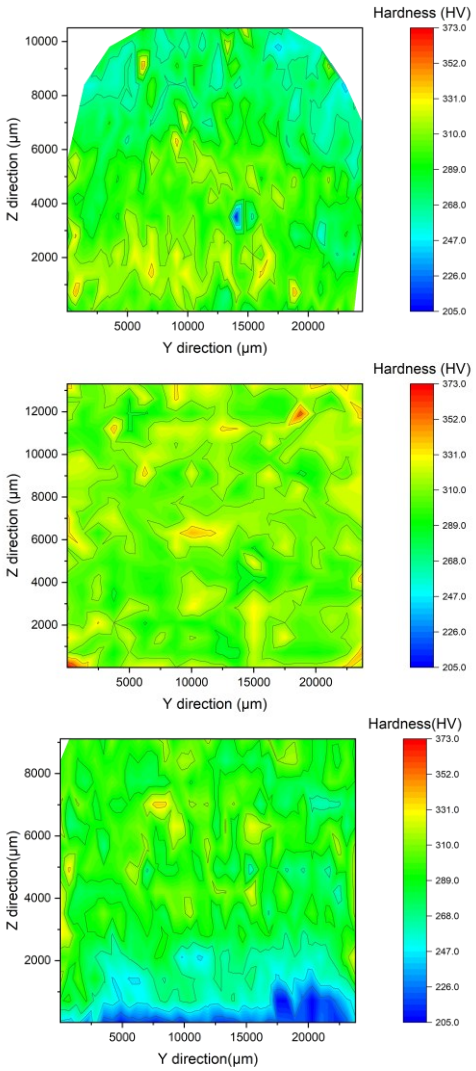


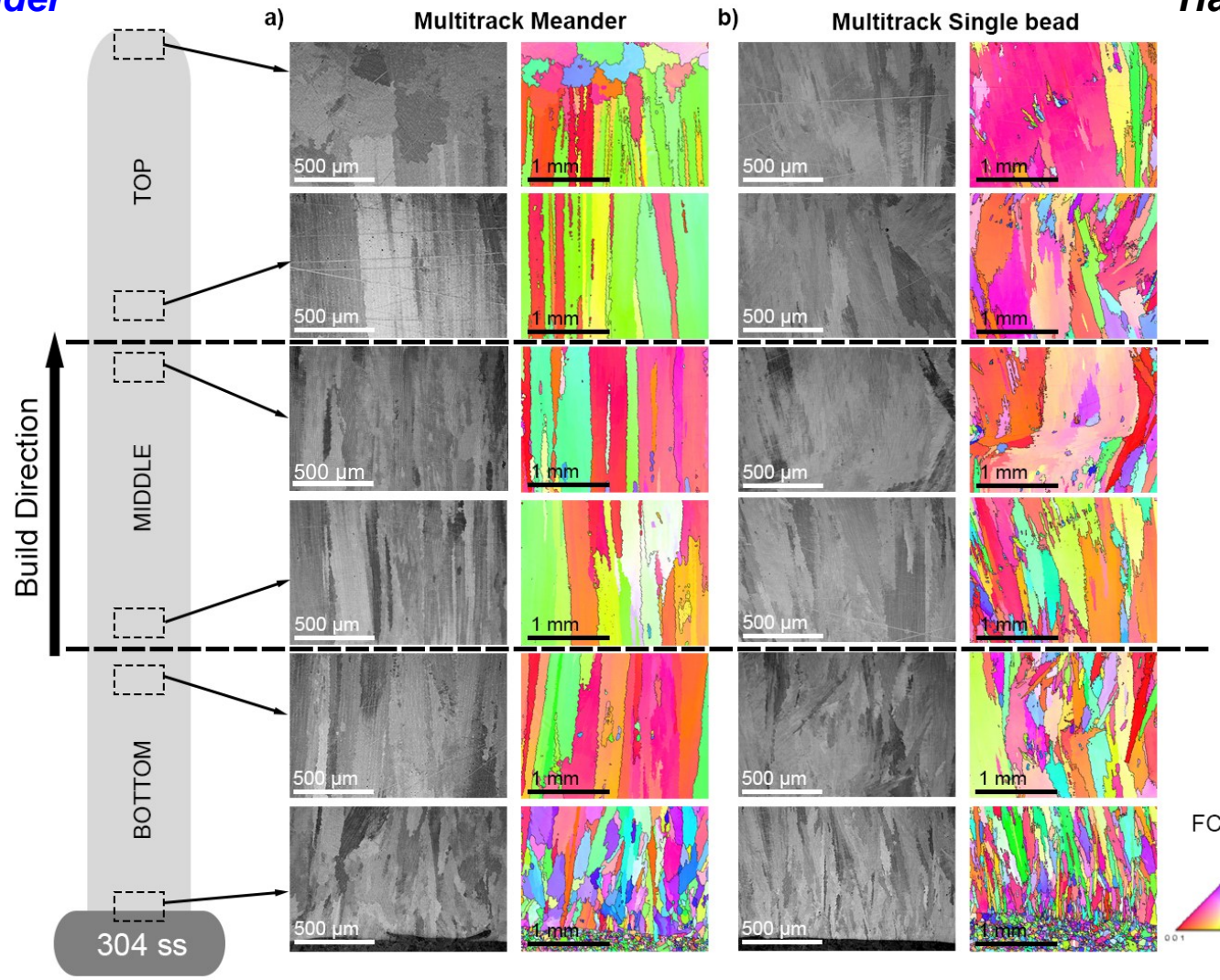
Zig-zag (meander)



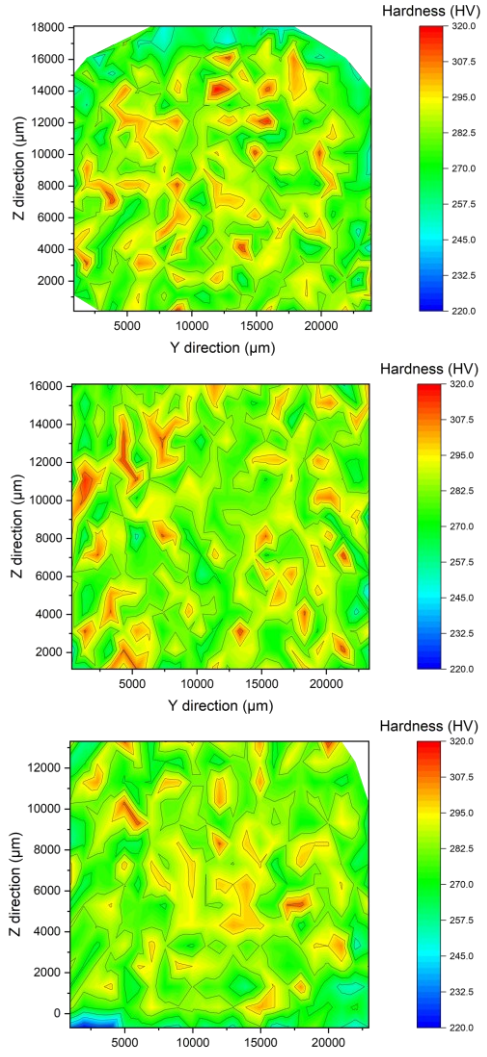
As-printed microstructure: Meander vs. Single Bead

Hardness Map of Meander



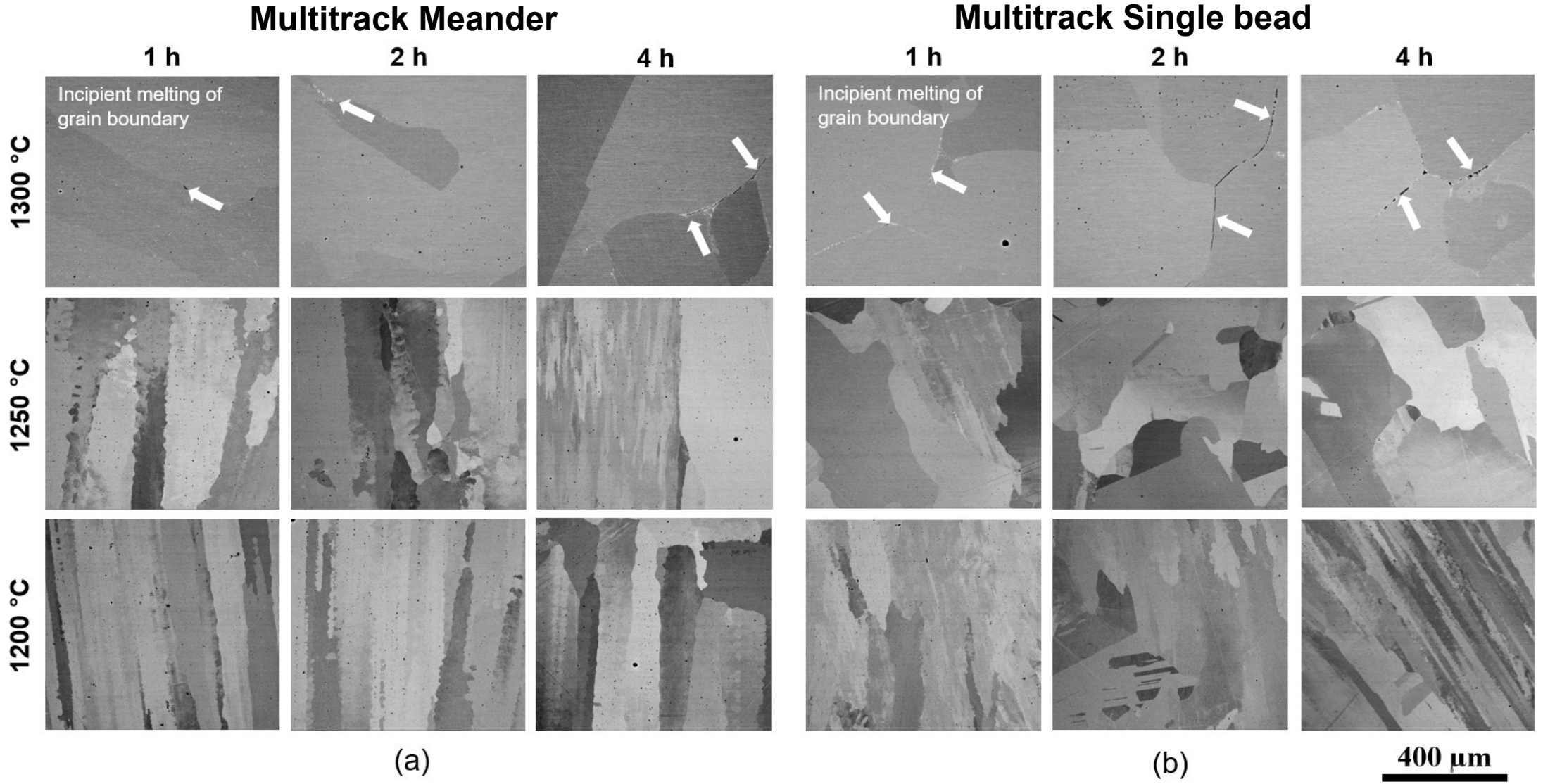


Hardness Map of Single Bead



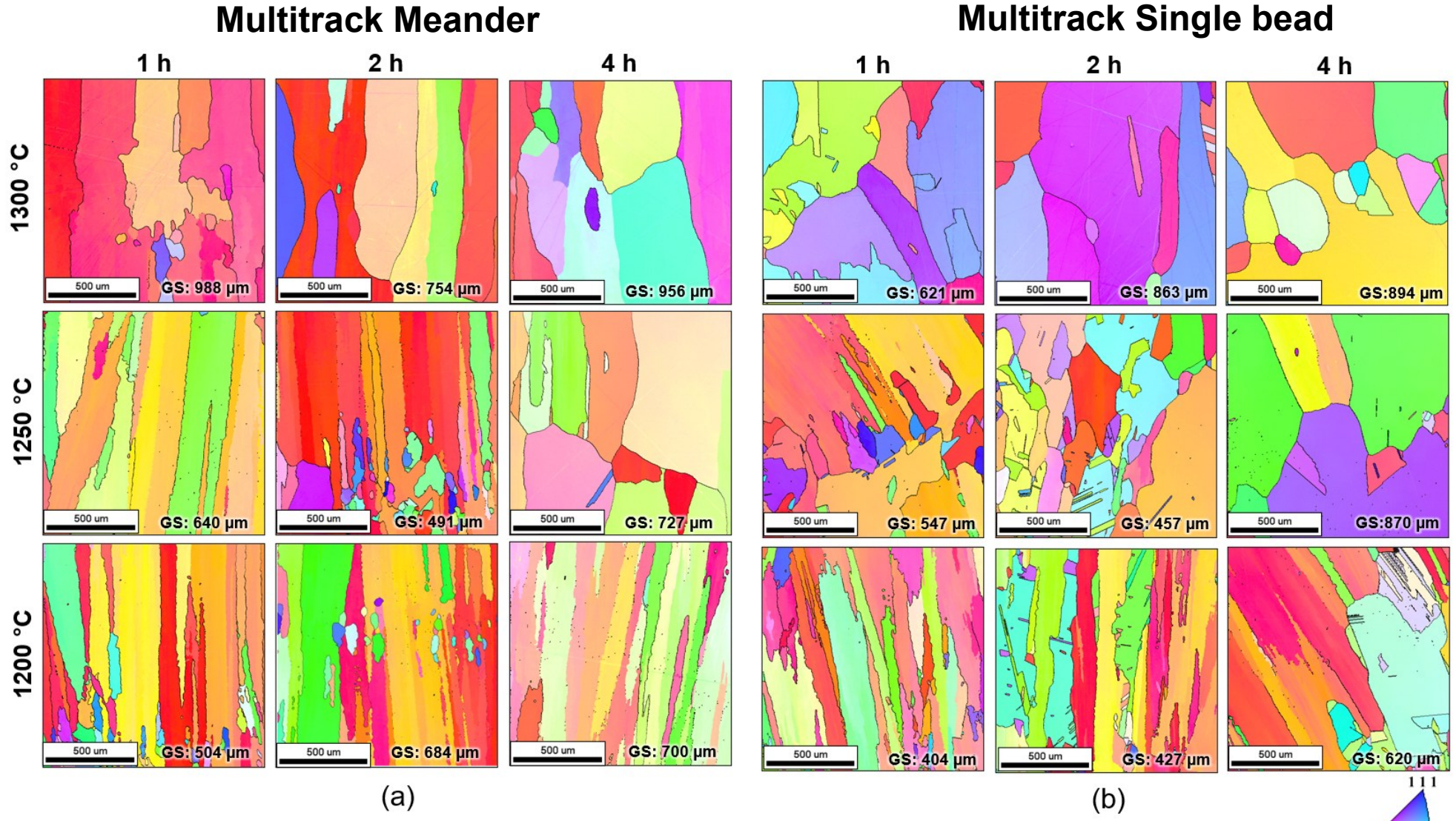
Luis Fernando Ladinos Pizano, Soumya Sridar, Rafael Rodriguez De Vecchis, Xin Wang, Jacob Biddlecom, Garrett J. Pataky, Chantal Sudbrack, Wei Xiong, Journal of Manufacturing Processes, 119 (2024) 781–789, https://doi.org/10.1016/j.jmapro.2024.04.015

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



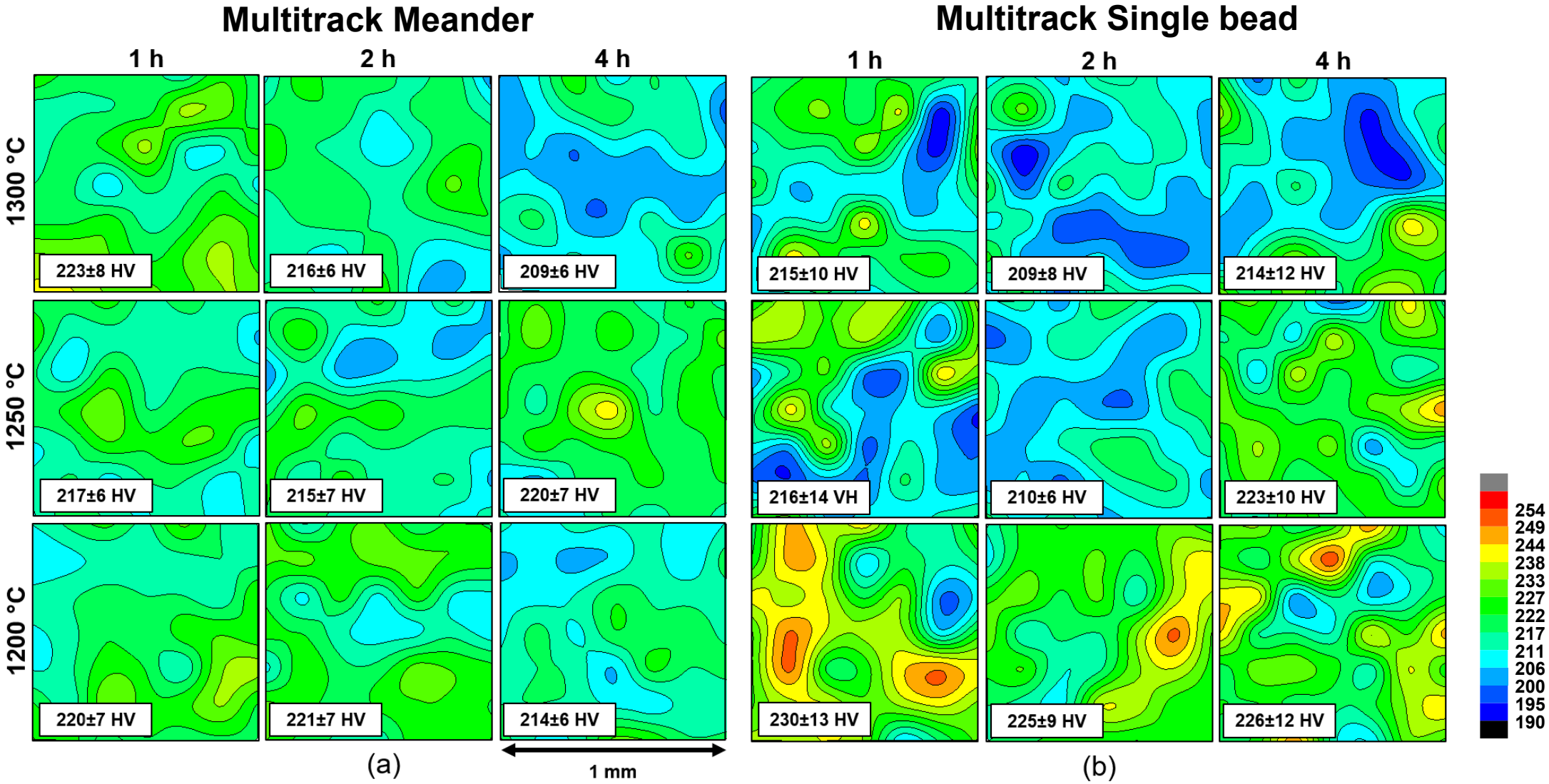
Luis Fernando Ladinos Pizano, Soumya Sridar, Rafael Rodriguez De Vecchis, Xin Wang, Jacob Biddlecom, Garrett J. Pataky, Chantal Sudbrack, Wei Xiong, Journal of Manufacturing Processes, 119 (2024) 781–789, https://doi.org/10.1016/j.jmapro.2024.04.015

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



Luis Fernando Ladinos Pizano, Soumya Sridar, Rafael Rodriguez De Vecchis, Xin Wang, Jacob Biddlecom, Garrett J. Pataky, Chantal Sudbrack, Wei Xiong, Journal of Manufacturing Processes, 119 (2024) 781–789, https://doi.org/10.1016/j.jmapro.2024.04.015

Recrystallization studies for build: **Hardness**



Luis Fernando Ladinos Pizano, Soumya Sridar, Rafael Rodriguez De Vecchis, Xin Wang, Jacob Biddlecom, Garrett J. Pataky, Chantal Sudbrack, Wei Xiong, Journal of Manufacturing Processes, 119 (2024) 781–789, https://doi.org/10.1016/j.jmapro.2024.04.015

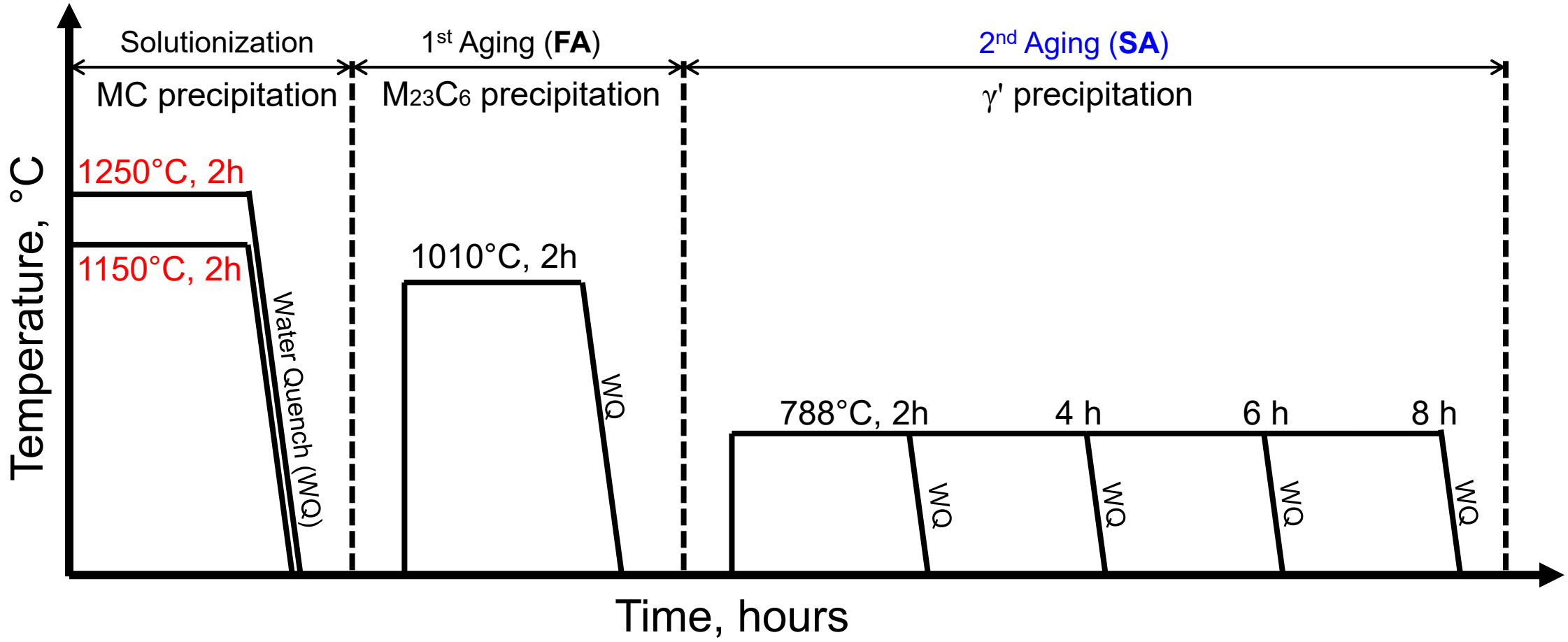
Summary of recrystallization studies

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

Effect of solution heat treatment on γ' precipitation

Luis Fernando Ladinos Pizano, Chantal Sudbrack, Wei Xiong, CALPHAD-based ICME design of single-step aging to enhance mechanical strength of WAAM Haynes 282, Materials Science and Engineering: A, 947 (2025) 149234, https://doi.org/10.1016/j.msea.2025.149234



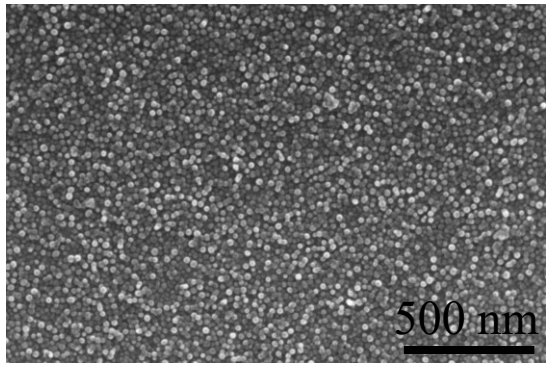
- The effect of solution temperature and aging time on gamma prime precipitation was systematically studied.
- FA and SA mean first and second aging, respectively.

Effect of solution heat treatment on γ' precipitation

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

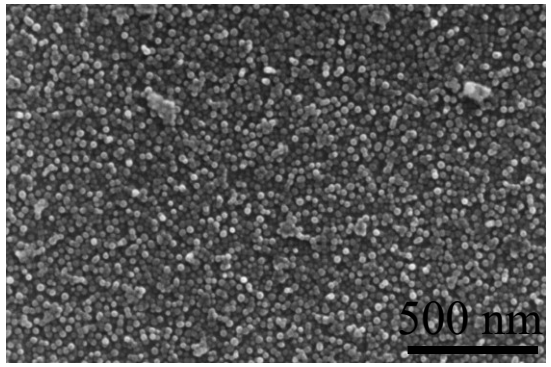
(a) **1250-FA-SA *x*h**

2h



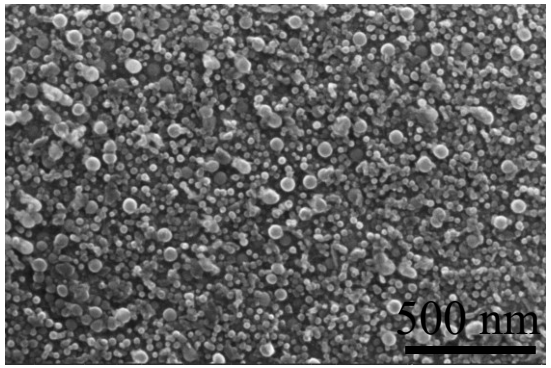
20.32 ± 3.08 nm

4h



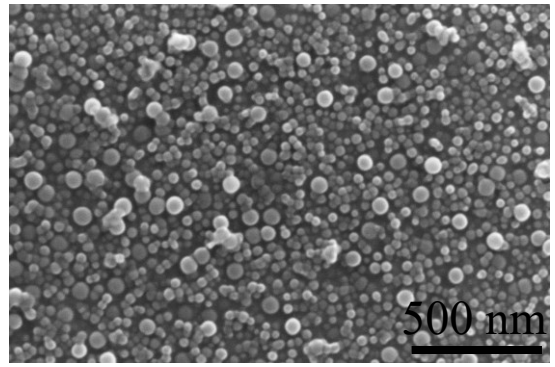
22.73 ± 4.62 nm

6h



25.59 ± 4.60 nm

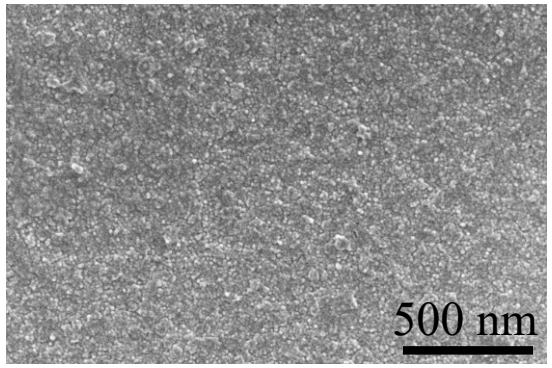
8h



30.73 ± 7.36 nm

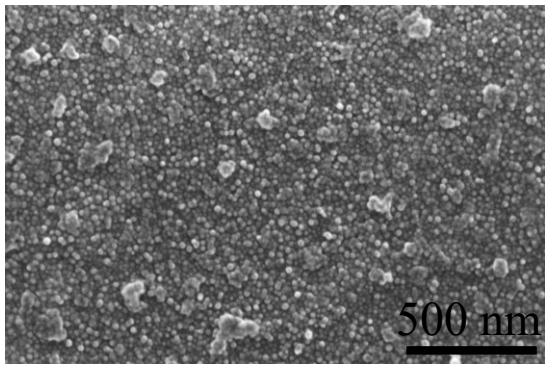
(b) **1150-FA-SA *x*h**

2h



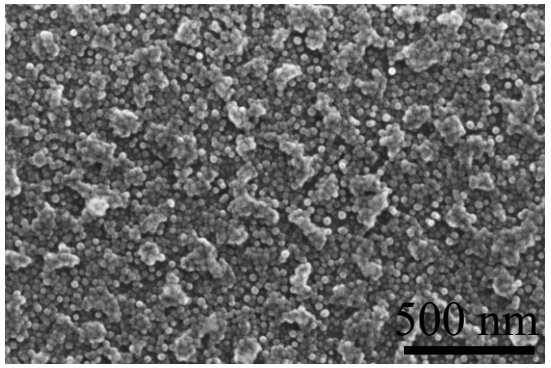
12.95 ± 1.34 nm

4h



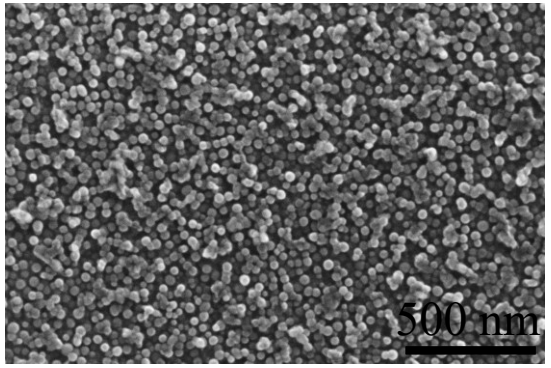
17.92 ± 4.01 nm

6h



25.42 ± 2.04 nm

8h



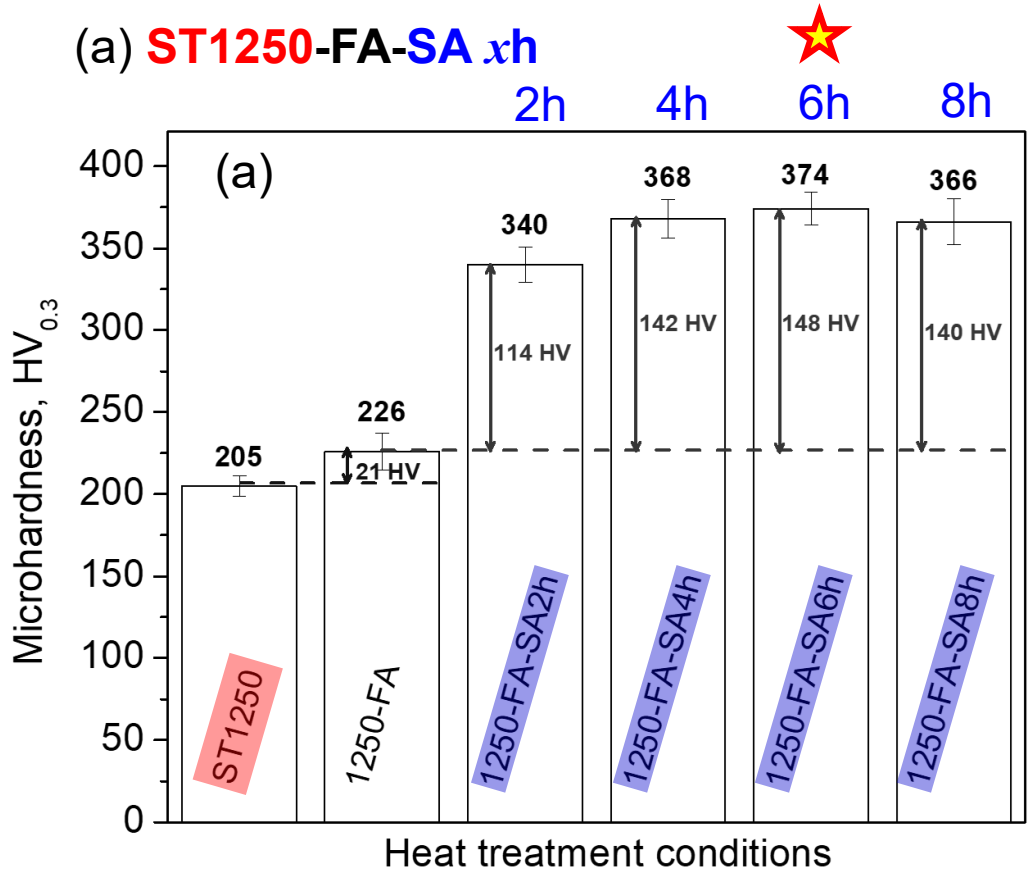
28.19 ± 2.73 nm

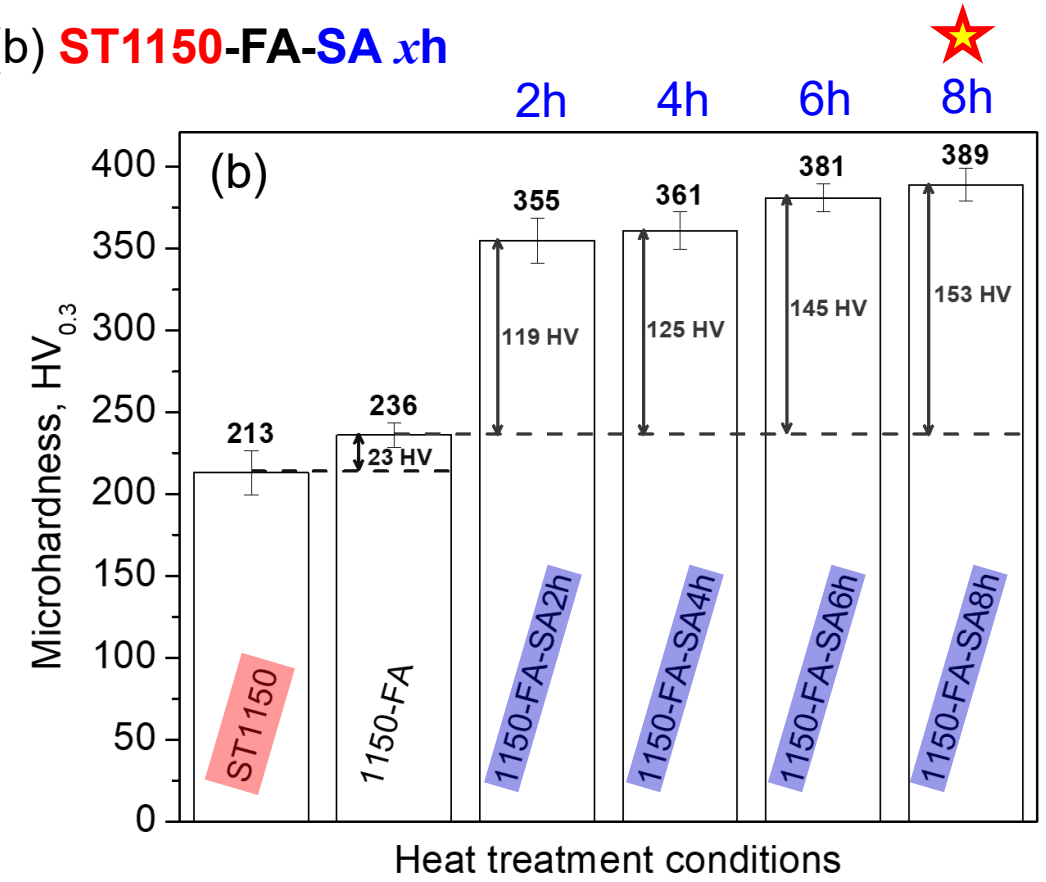
Luis Fernando Ladinos Pizano, Chantal Sudbrack, Wei Xiong, CALPHAD-based ICME design of single-step aging to enhance mechanical strength of WAAM Haynes 282, Materials Science and Engineering: A, 947 (2025) 149234, https://doi.org/10.1016/j.msea.2025.149234

Hardness evolution

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

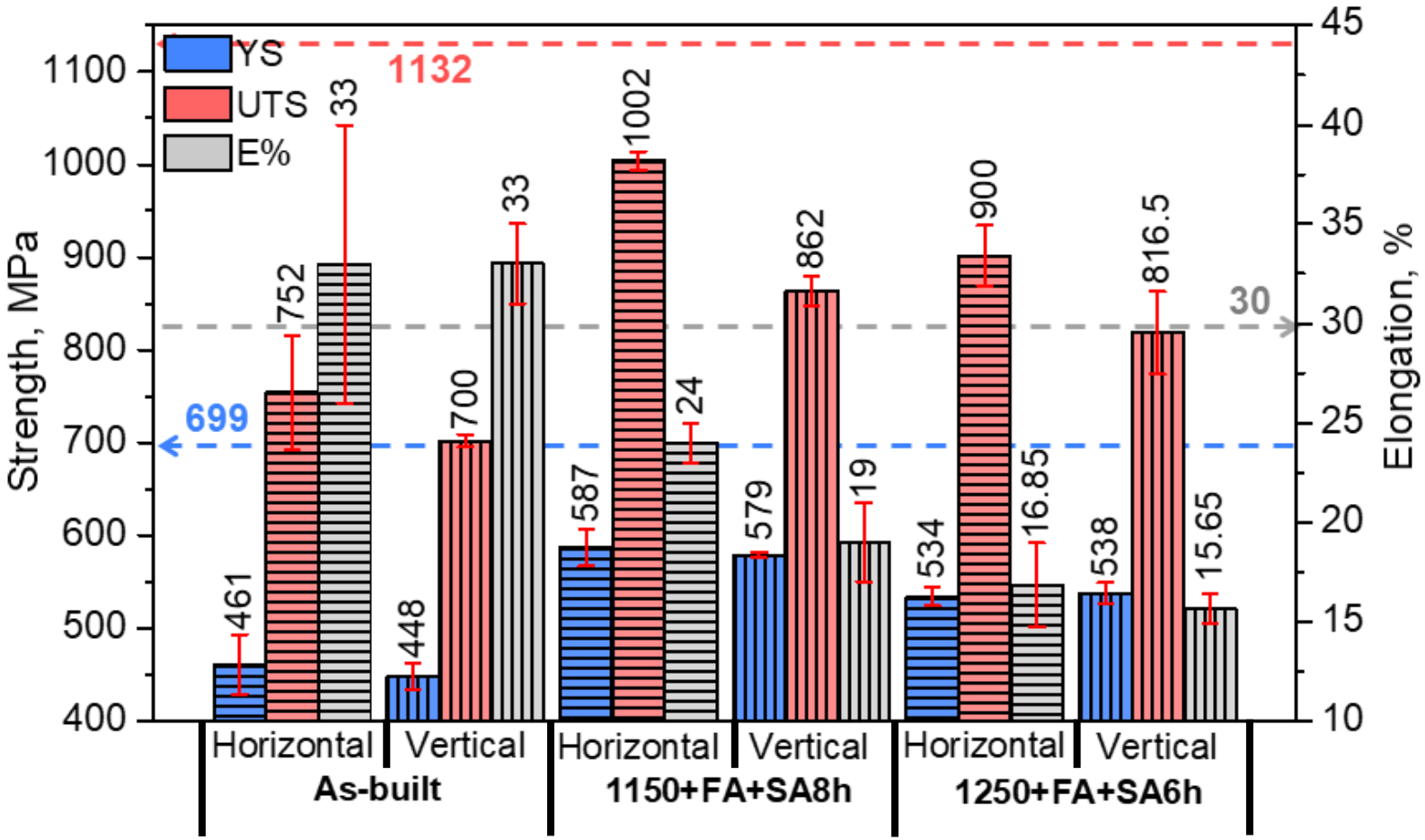
- The hardness peak is achieved slightly faster in samples exposed to 1250°C during solution heat treatment.
- The hardness of samples 1150-FA-SA8h and 1250-FA-SA6h show a hardness **similar to** the hardness of Haynes 282 made by forging (373 HV)





Luis Fernando Ladinos Pizano, Chantal Sudbrack, Wei Xiong, CALPHAD-based ICME design of single-step aging to enhance mechanical strength of WAAM Haynes 282, Materials Science and Engineering: A, 947 (2025) 149234, https://doi.org/10.1016/j.msea.2025.149234

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.

Luis Fernando Ladinos Pizano, Chantal Sudbrack, Wei Xiong, CALPHAD-based ICME design of single-step aging to enhance mechanical strength of WAAM Haynes 282, Materials Science and Engineering: A, 947 (2025) 149234, https://doi.org/10.1016/j.msea.2025.149234

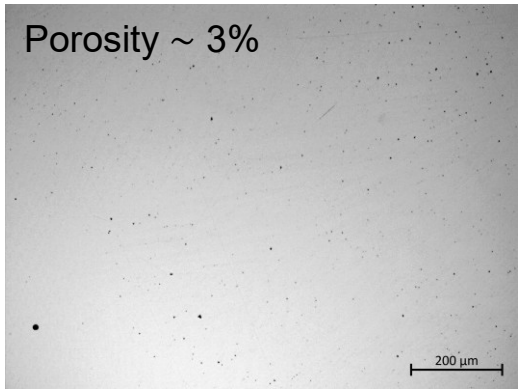
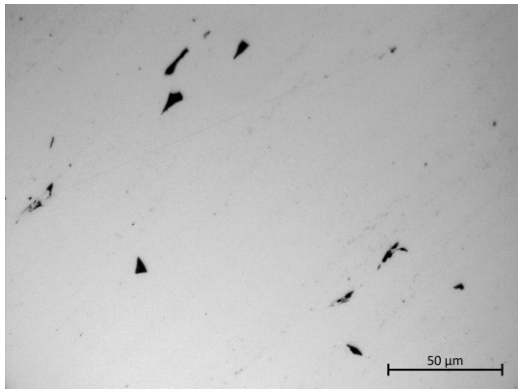
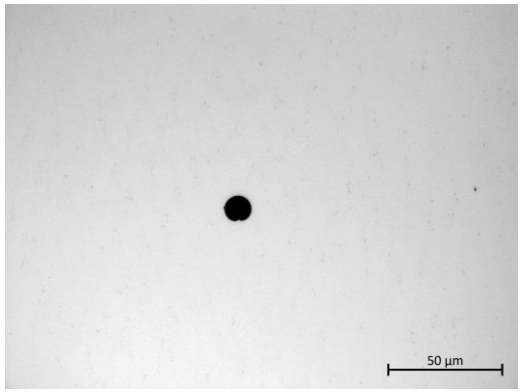
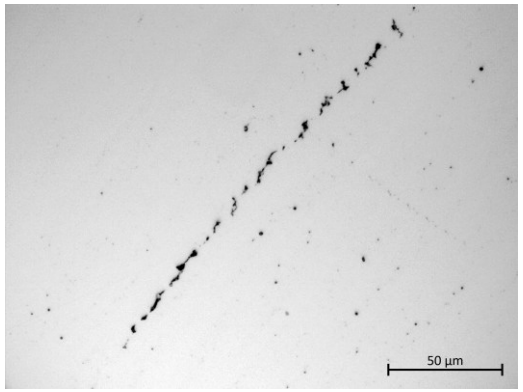
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Why we have even worse yield strength with high hardness?

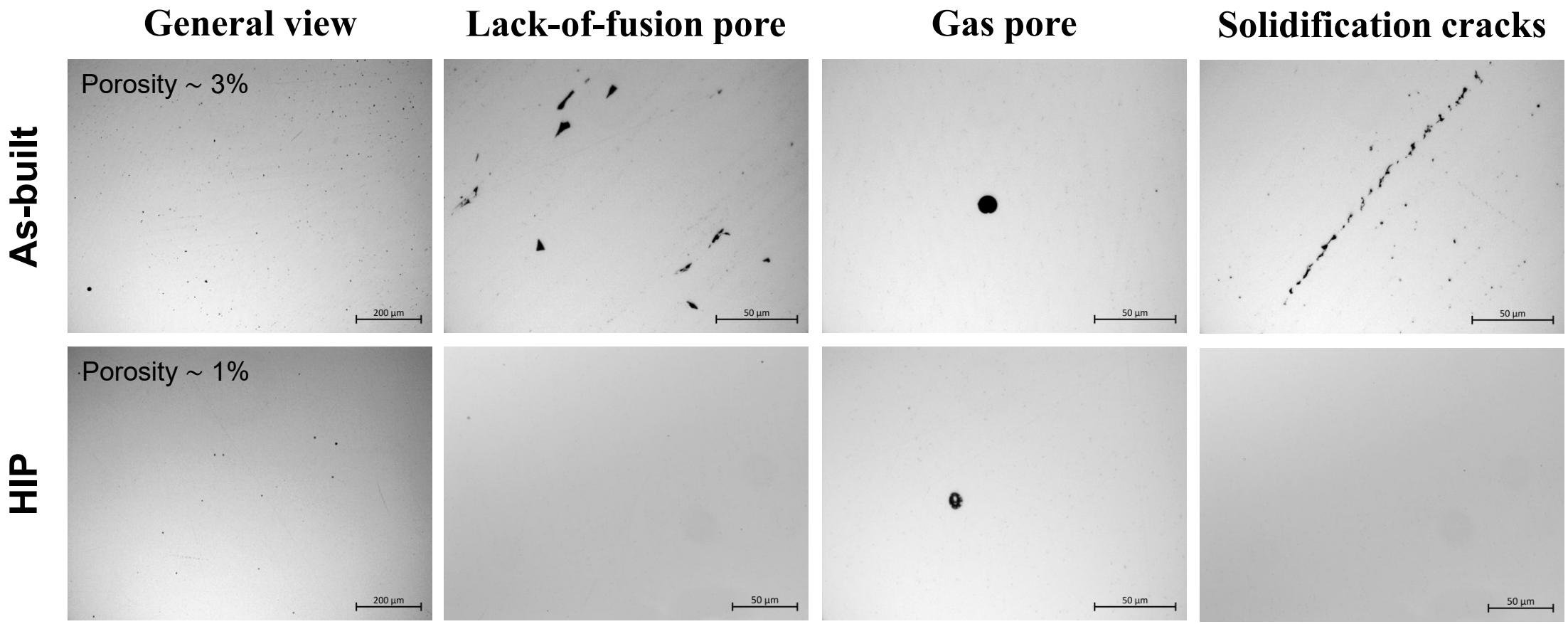


Porosity: as-built condition

	General view	Lack-of-fusion pore	Gas pore	Solidification cracks
As-built				

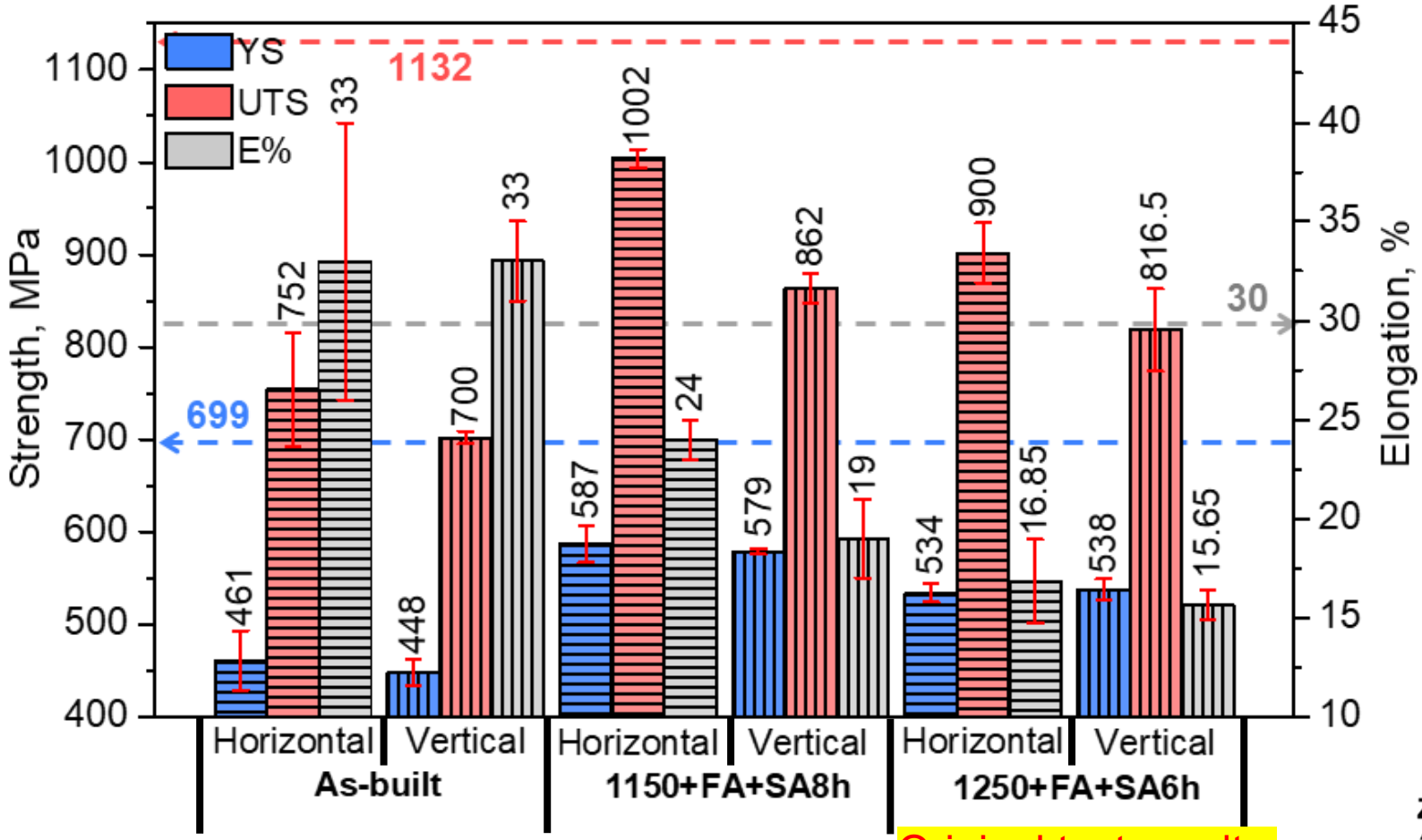
- As-built samples show porosity due to lack of fusion and gas. In addition, cracks of solidification were located.

Porosity before and after HIP

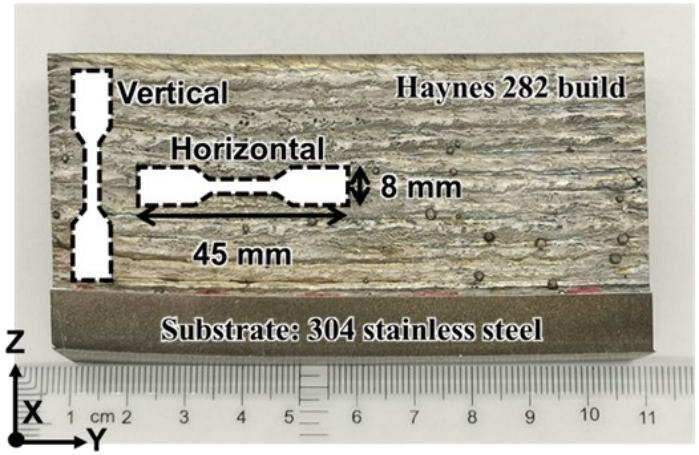


- As-built samples show porosity due to lack of fusion and gas. In addition, cracks of solidification were located.
- Samples after HIP show only gas pores.

Tensile test on samples w/o HIP



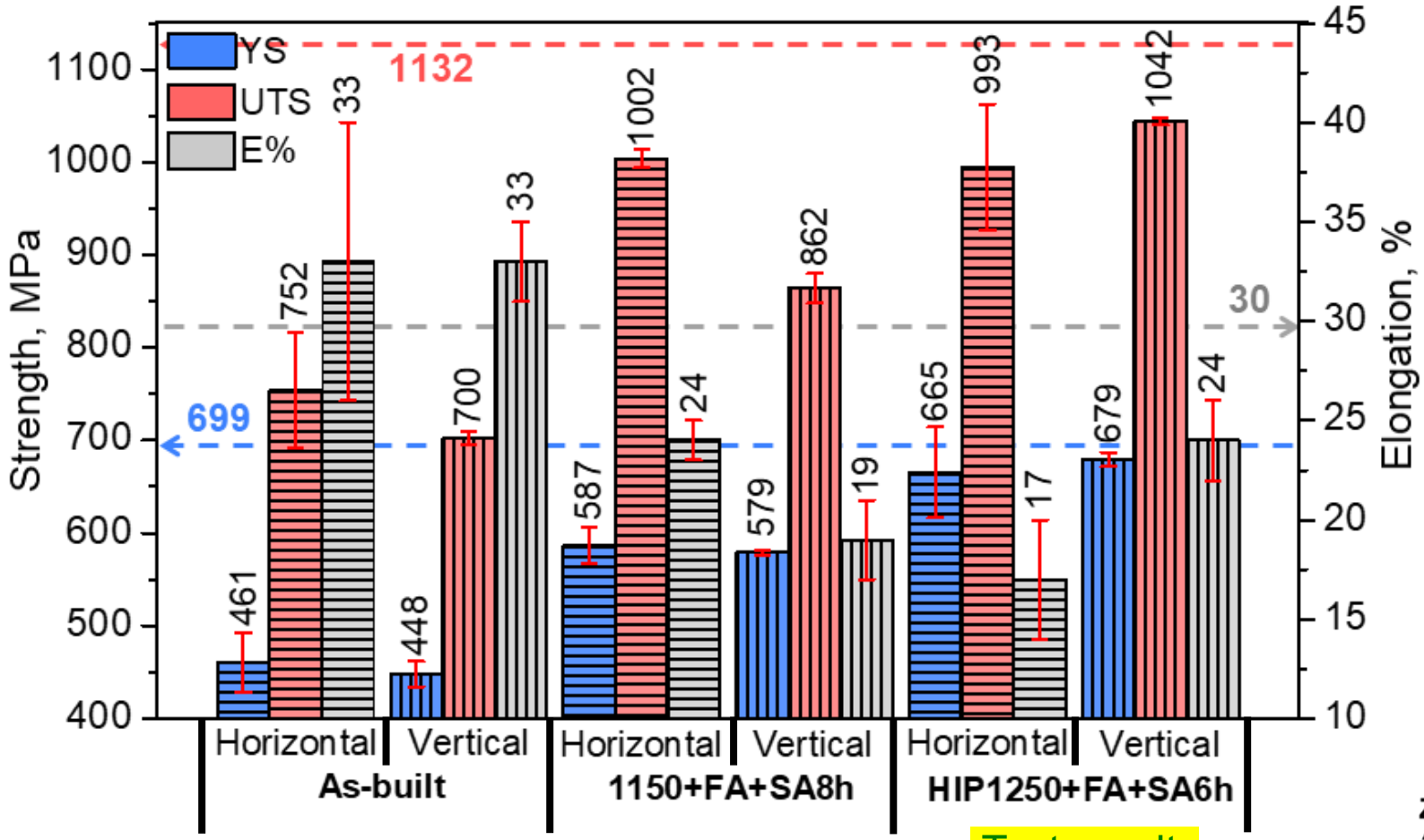
Original test results w/o HIP



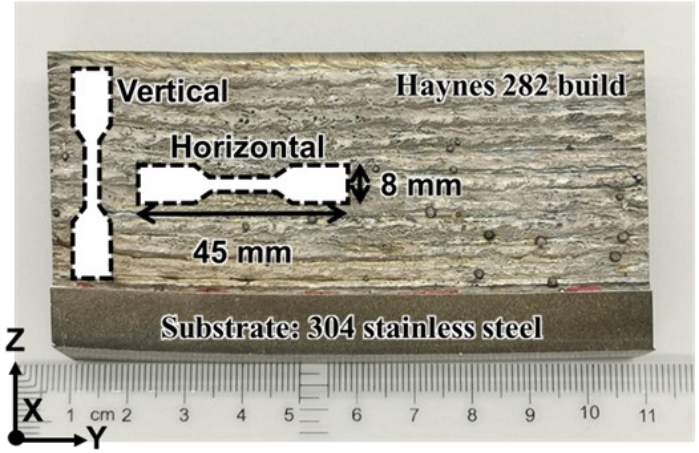
Luis Fernando Ladinos Pizano, Chantal Sudbrack, Wei Xiong, CALPHAD-based ICME design of single-step aging to enhance mechanical strength of WAAM Haynes 282, Materials Science and Engineering: A, 947 (2025) 149234, https://doi.org/10.1016/j.msea.2025.149234

FA: First aging, SA: Second aging

Tensile test on samples with HIP



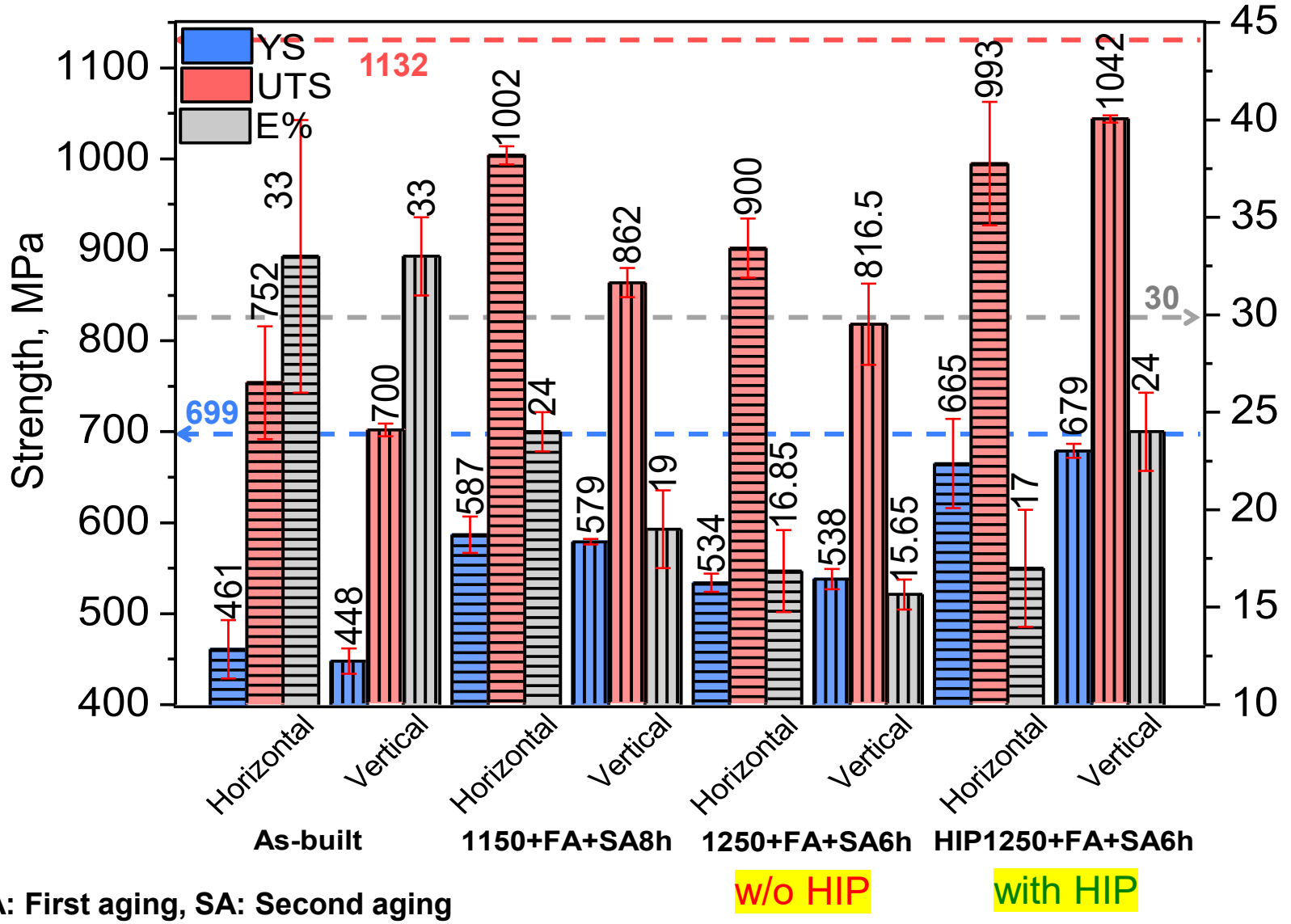
Test results with HIP



Luis Fernando Ladinos Pizano, Chantal Sudbrack, Wei Xiong, CALPHAD-based ICME design of single-step aging to enhance mechanical strength of WAAM Haynes 282, Materials Science and Engineering: A, 947 (2025) 149234, https://doi.org/10.1016/j.msea.2025.149234

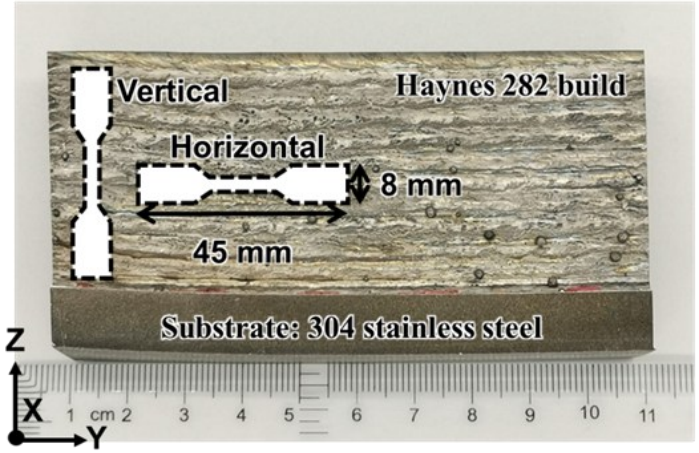
FA: First aging, SA: Second aging

Tensile test with vs. without HIP



FA: First aging, SA: Second aging

Luis Fernando Ladinos Pizano, Chantal Sudbrack, Wei Xiong, CALPHAD-based ICME design of single-step aging to enhance mechanical strength of WAAM Haynes 282, Materials Science and Engineering: A, 947 (2025) 149234, https://doi.org/10.1016/j.msea.2025.149234

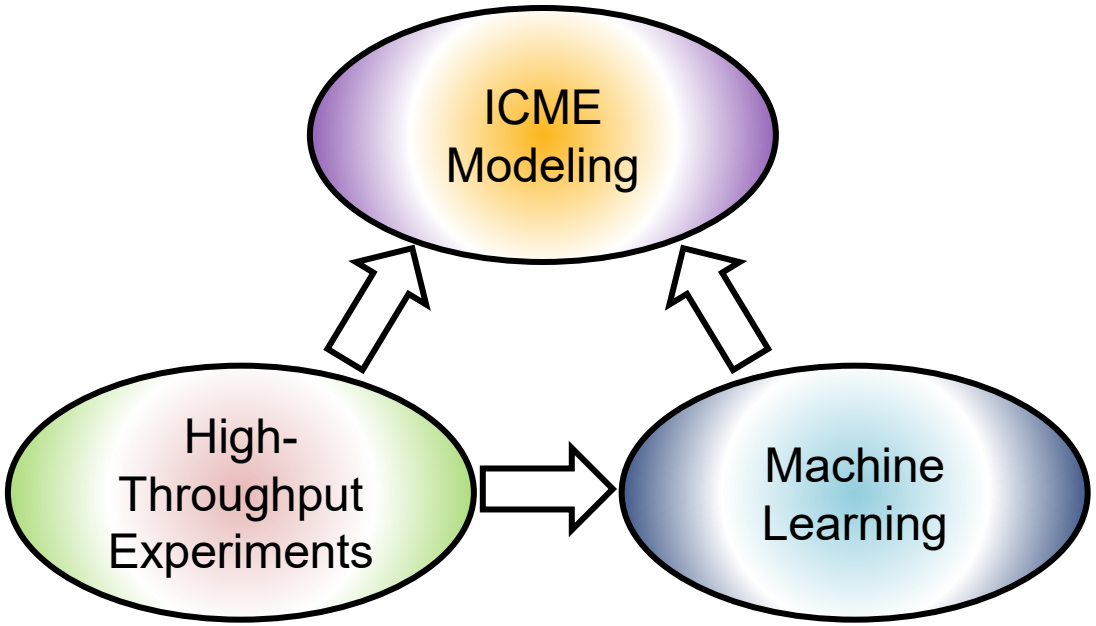


PMMD

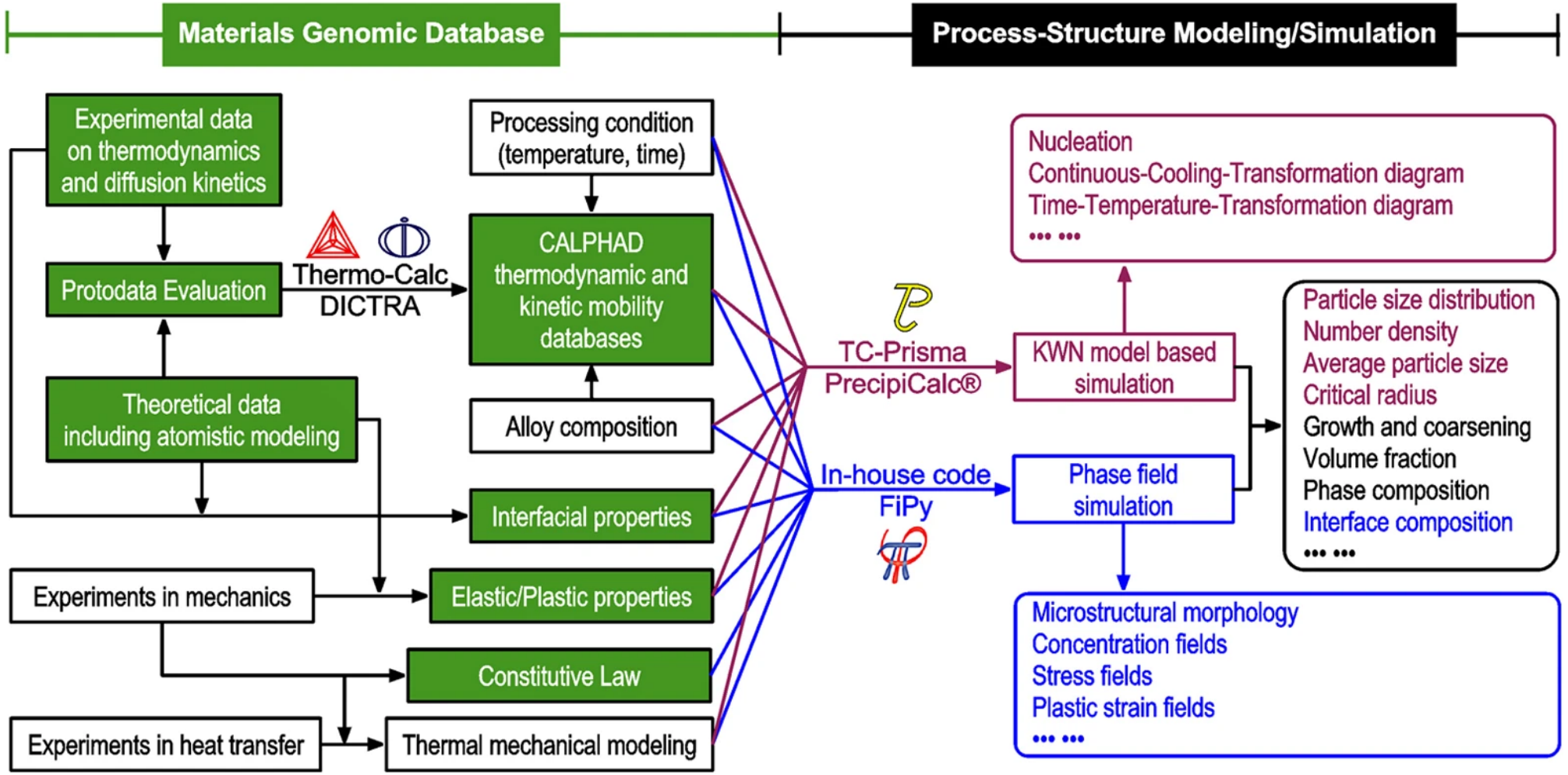
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ICME design modeling from microstructure to strength properties

high-throughput experiment and machine learning

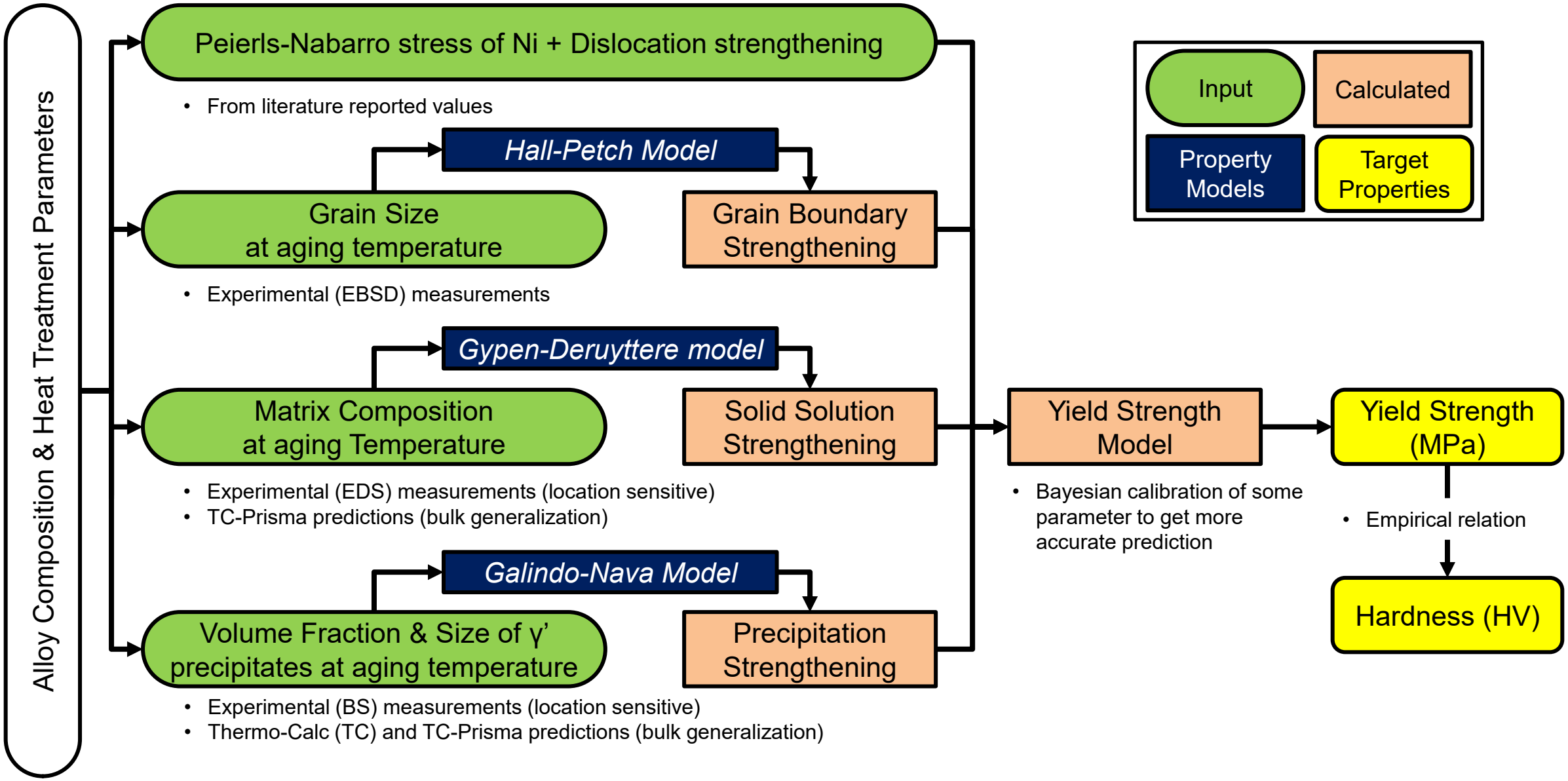


CALPHAD-based ICME modeling of precipitation kinetics

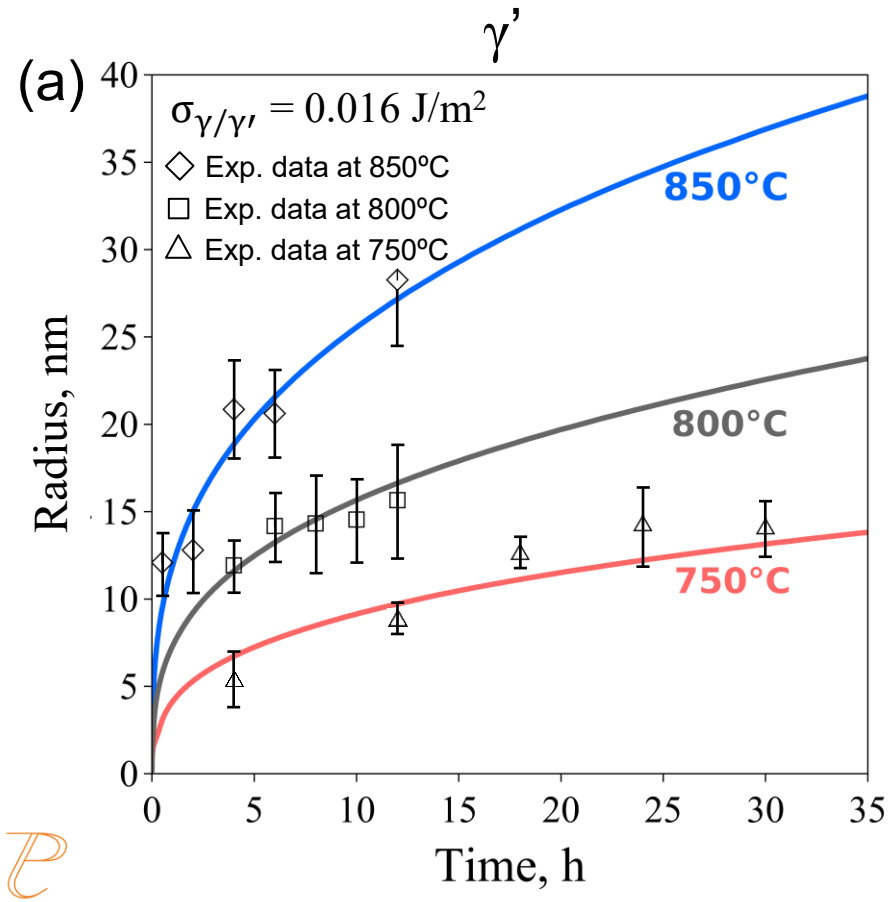


Wei Xiong, Gregory B. Olson, ***npj Computational Materials***, 2 (2016) 15009.

ICME Yield Strength Model Overview



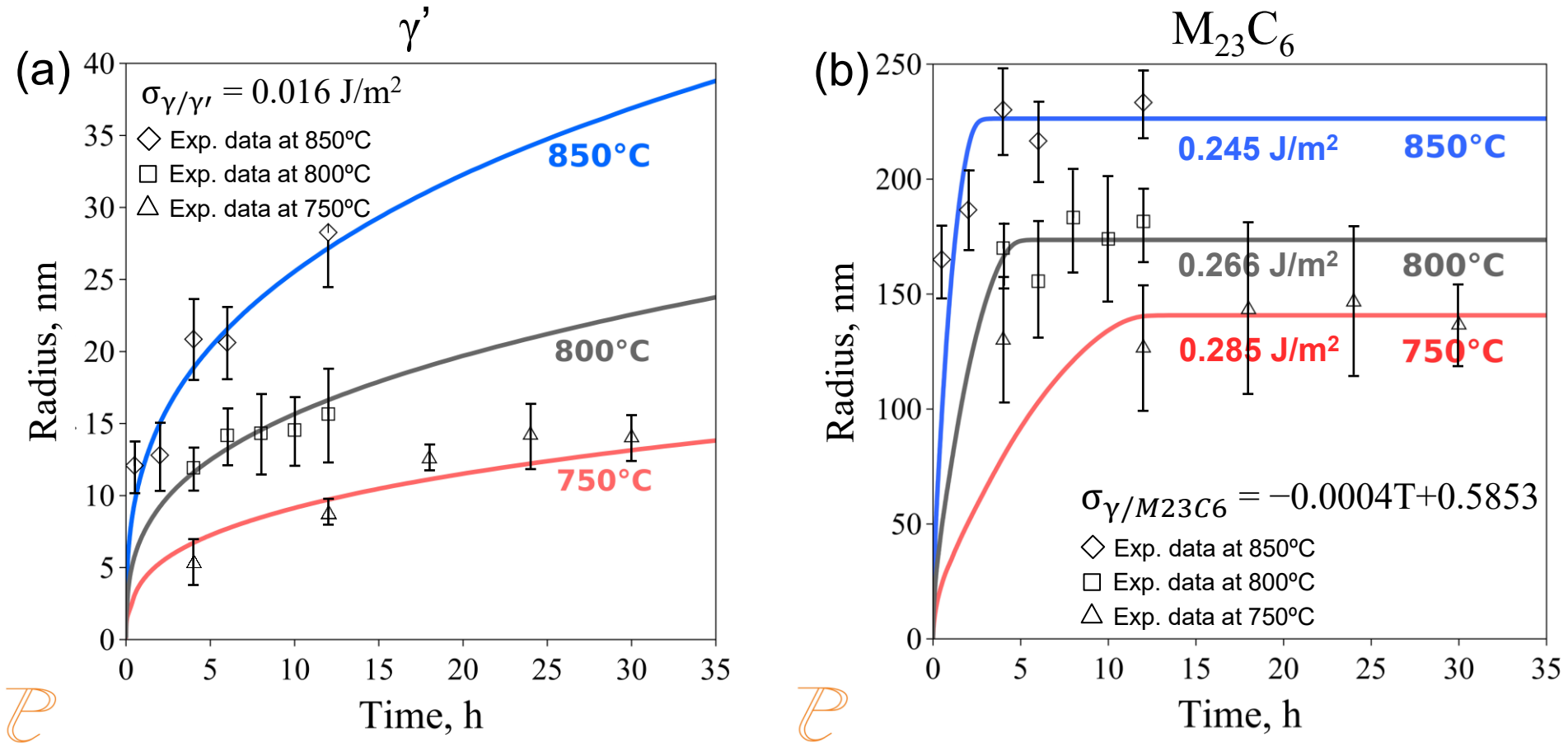
Estimation of the interfacial energy of γ/γ’ and γ/M23C6.



- Coarsening curves of γ’ as a function of temperature (750, 800 and 850°C) and time (0 to 35h) were calculated using TC-Prisma and the thermodynamic and mobility databases TCNI11 and MOBNI5.
- The simulation considers spherical morphologies for both precipitates.
- The experimental data are represented by the black points and were used to fit the coarsening curves.
- Based on this analysis, the interfacial energy of γ/γ' was estimated at 0.016J/m2 in a temperature range of 750 to 850°C.

Luis Fernando Ladinos Pizano, Chantal Sudbrack, Wei Xiong, CALPHAD-based ICME design of single-step aging to enhance mechanical strength of WAAM Haynes 282, **Materials Science and Engineering: A**, Volume 947, 2025, 149234, https://doi.org/10.1016/j.msea.2025.149234.

Estimation of the interfacial energy of γ/γ’ and γ/M23C6.

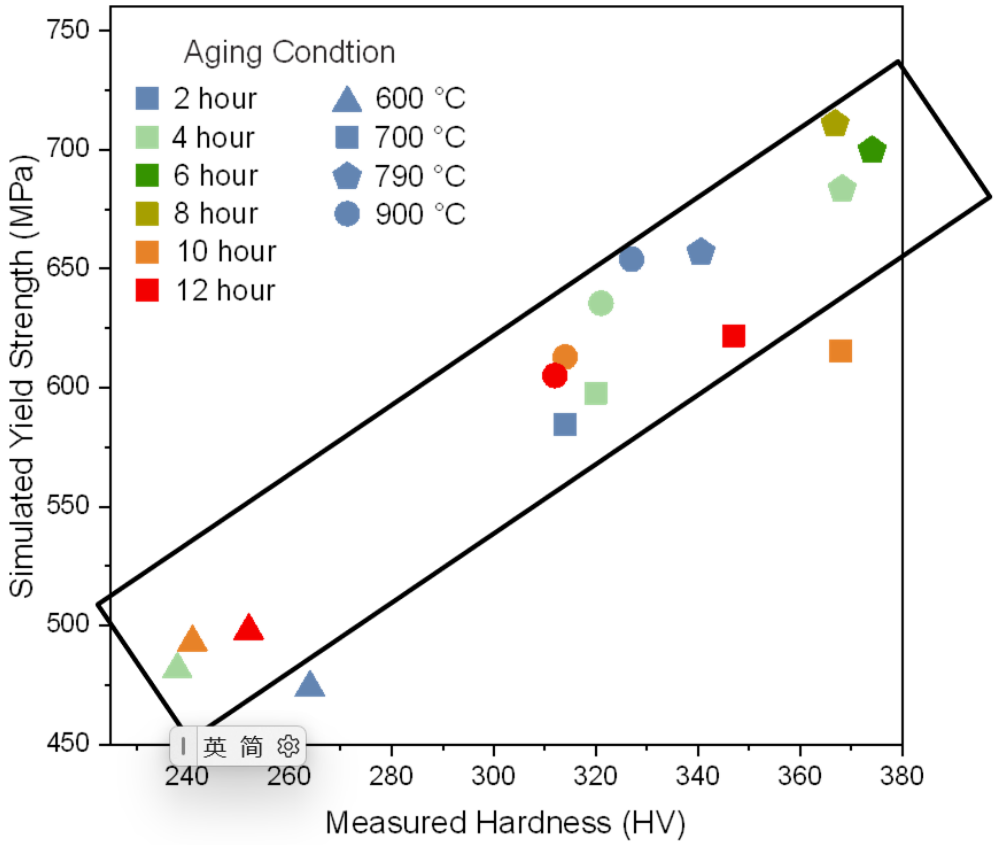


- The interfacial energy of γ/M23C6 varies from 0.245 to 0.285 in this temperature range.
- The equation in figure (b) represents the interfacial energy of γ /M23C6 as a function of temperature which is used in the high-throughput simulation to predict the precipitation behavior of these carbides.

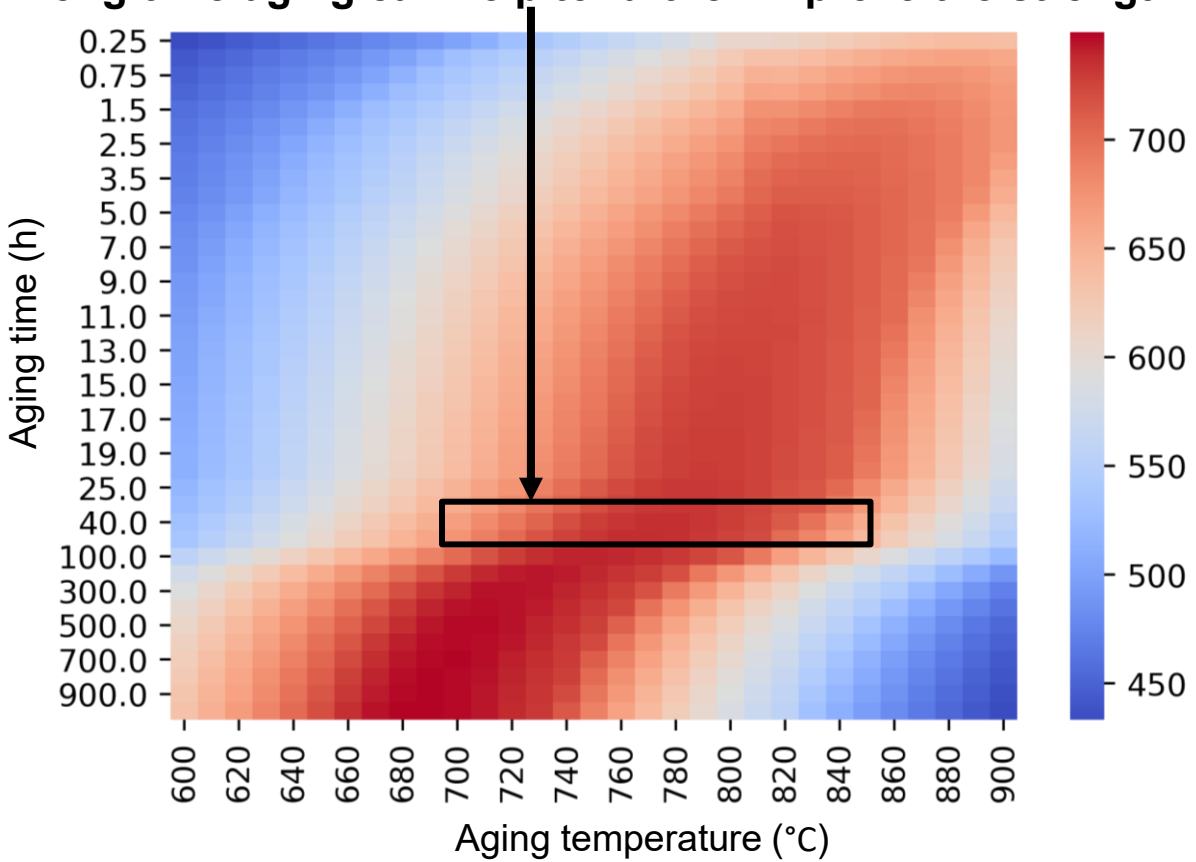
Interfacial Energy Calibration and Yield Strength Prediction

Simulation vs. Experiments:

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

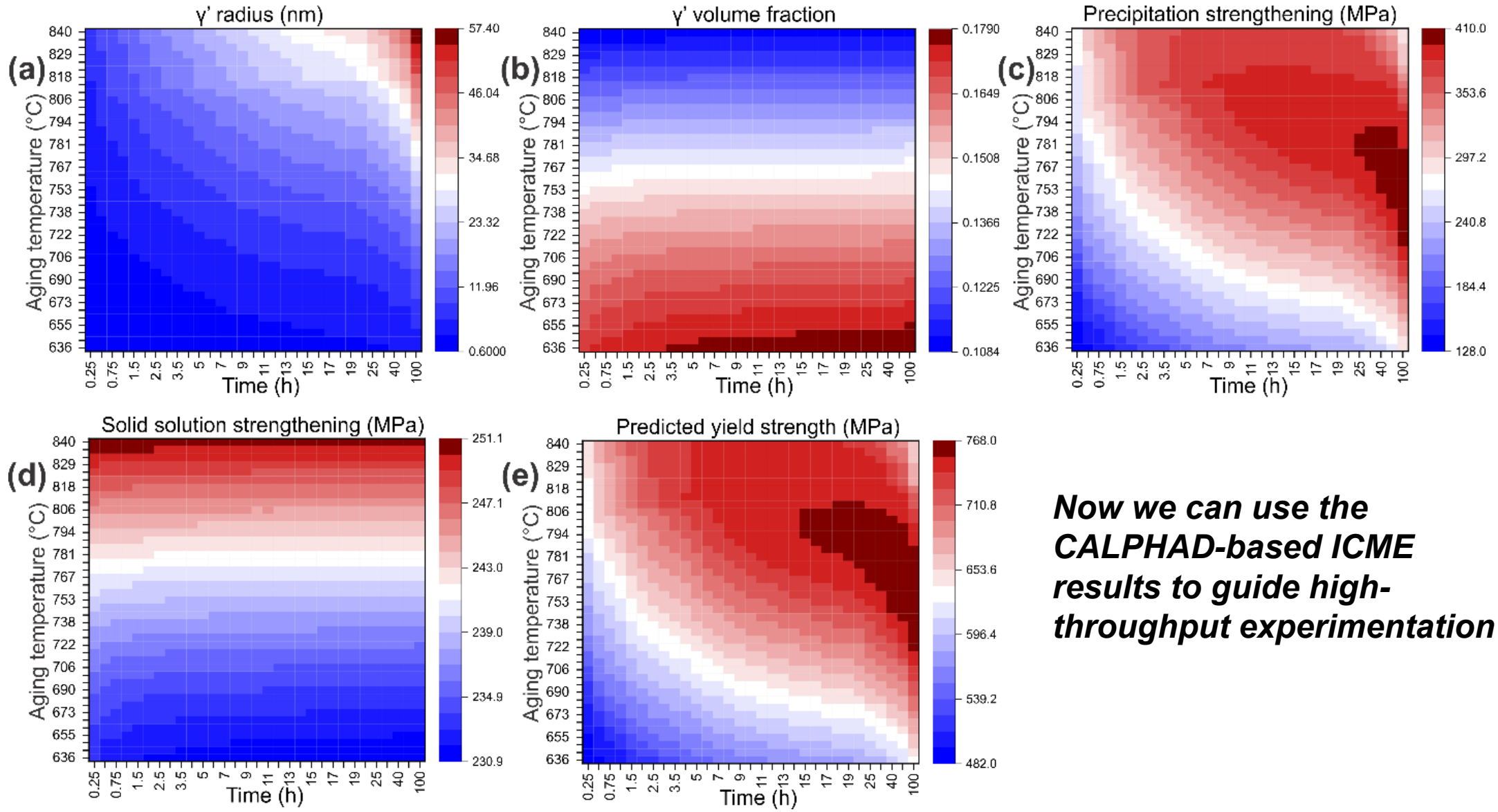


Desired yield strength can be achieved in less than 50 hours in the temperature range of 700-850°C, although long-time aging can help to further improve the strength.



Xin Wang, Luis Fernando Ladinos Pizano, Soumya Sridar, Chantal Sudbrack, Wei Xiong, ***Science and Technology of Advanced Materials***, 25(1) (2024) 2346067. DOI: 10.1080/14686996.2024.2346067

CALPHAD-based ICME model prediction after calibration using experiments



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

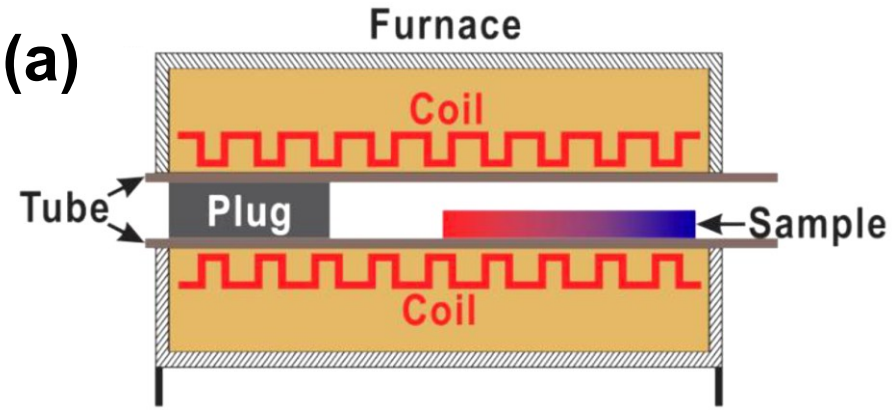
High-throughput experiments supporting ICME-ML design of yield strength

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

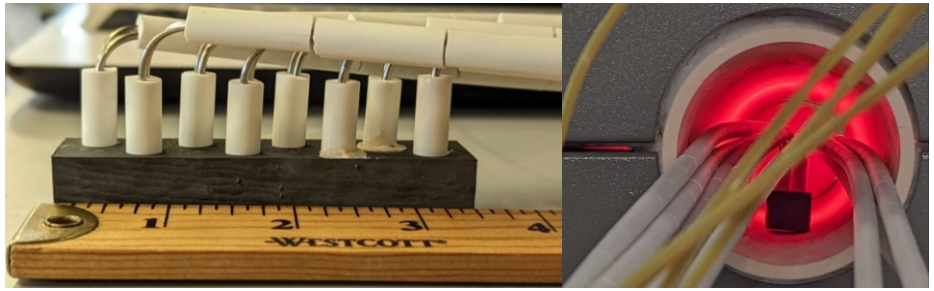
We applied HIP on high-throughput samples

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

(a)



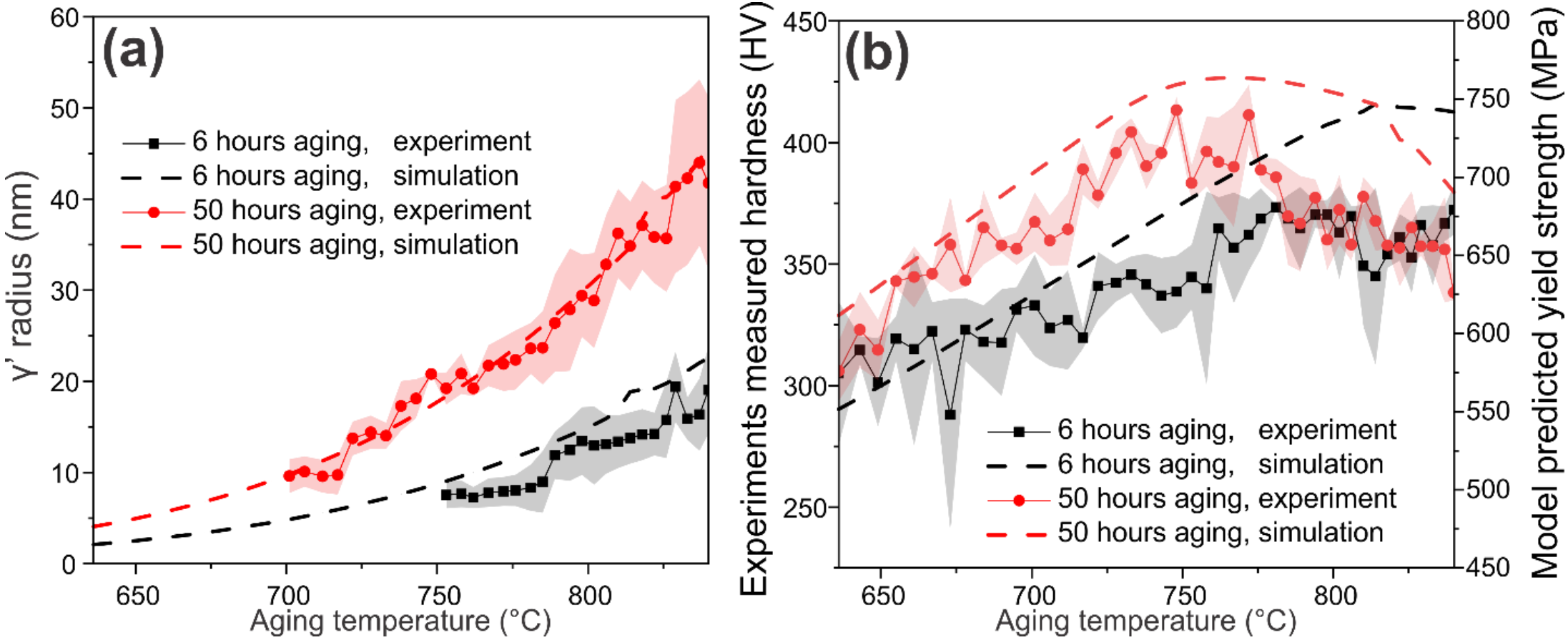
(b)



You can get microstructure information as many as you want to have with the fixed duration.

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

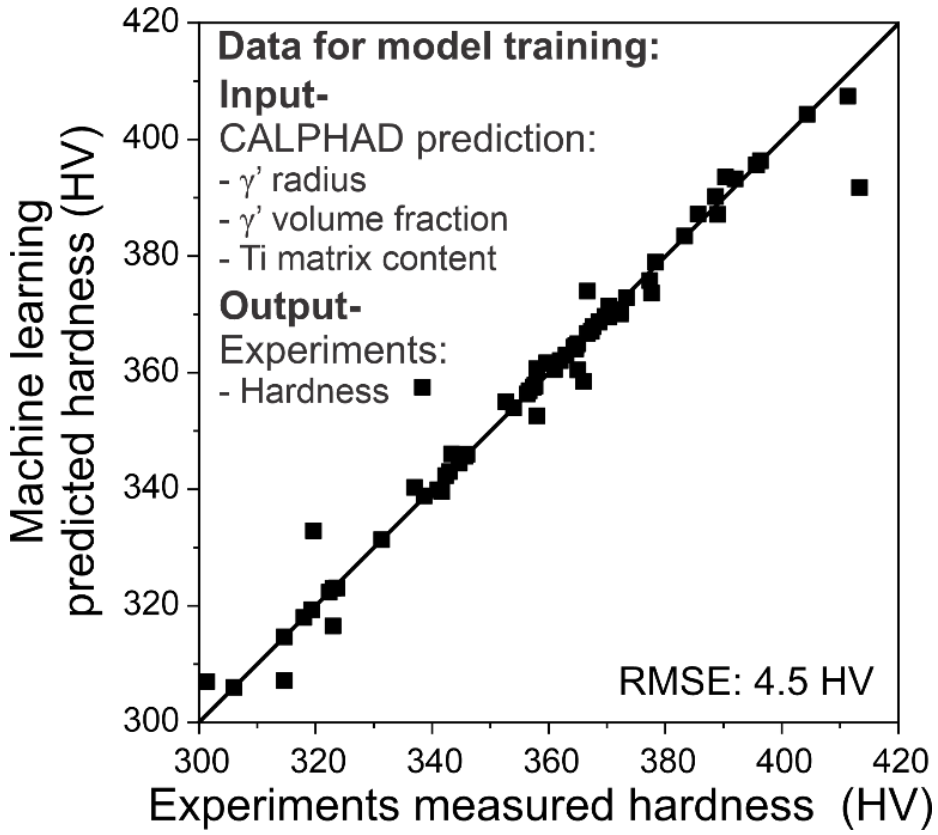
CALPHAD-based simulation of precipitation kinetics



Xin Wang, Luis Fernando Ladinos Pizano, Soumya Sridar, Chantal Sudbrack, Wei Xiong, ***Science and Technology of Advanced Materials***, 25(1) (2024) 2346067. DOI: 10.1080/14686996.2024.2346067

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

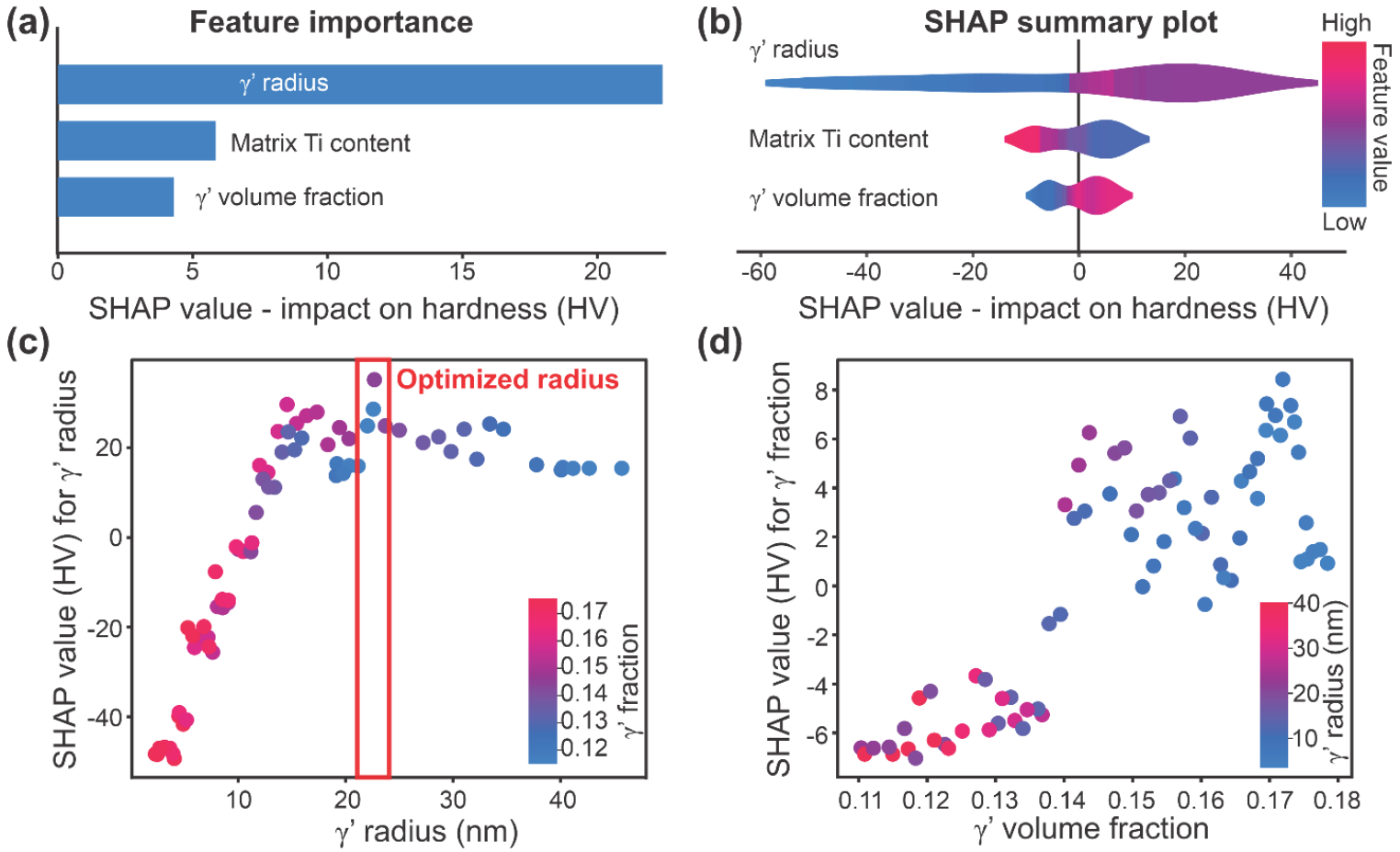
	Al	Co	Cr	Fe	Mn	Mo	Si	Ti	Ni
Al	1	-0.999	-0.999	-0.997	-0.999	-0.999	-0.998	0.996	0.999
Co	-0.999	1	1	0.999	1	1	1	-0.999	-1
Cr	-0.999	1	1	0.999	1	1	1	-0.999	-1
Fe	-0.997	0.999	0.999	1	0.999	1	1	-1	-0.999
Mn	-0.999	1	1	0.999	1	1	1	-0.998	-1
Mo	-0.999	1	1	1	1	1	1	-0.999	-1
Si	-0.998	1	1	1	1	1	1	-0.999	-1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

Xin Wang, Luis Fernando Ladinos Pizano, Soumya Sridar, Chantal Sudbrack, Wei Xiong, ***Science and Technology of Advanced Materials***, 25(1) (2024) 2346067. DOI: 10.1080/14686996.2024.2346067

Interpret the machine learning model using SHAP and heat treatment design

SHAP (SHapley Additive exPlanations)

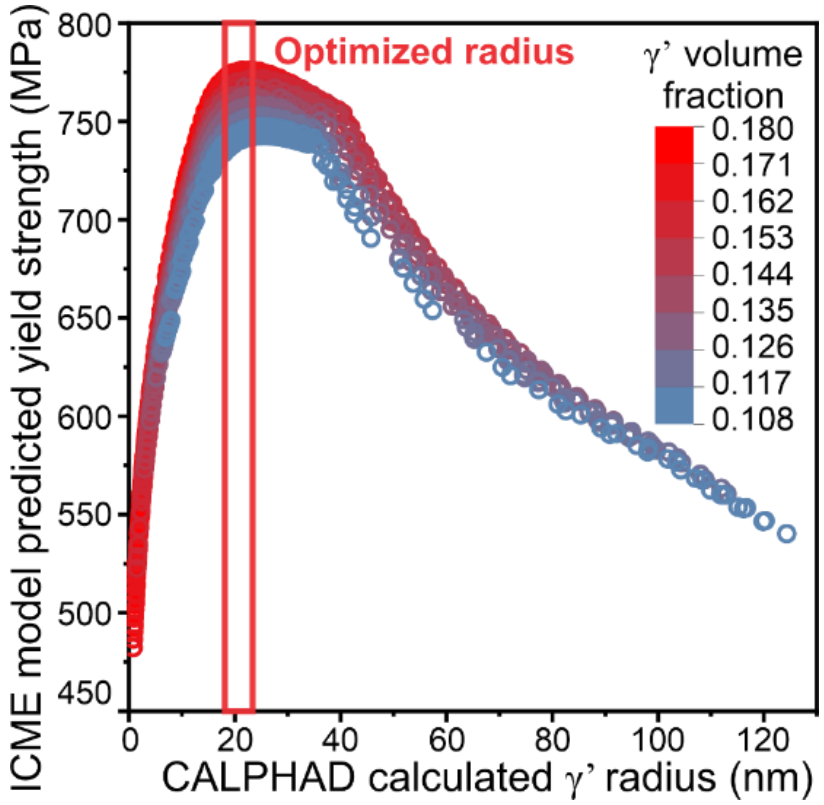
Phase fraction of γ' is less important than radius, as long as it reaches the desired range 14~18 vol.%.

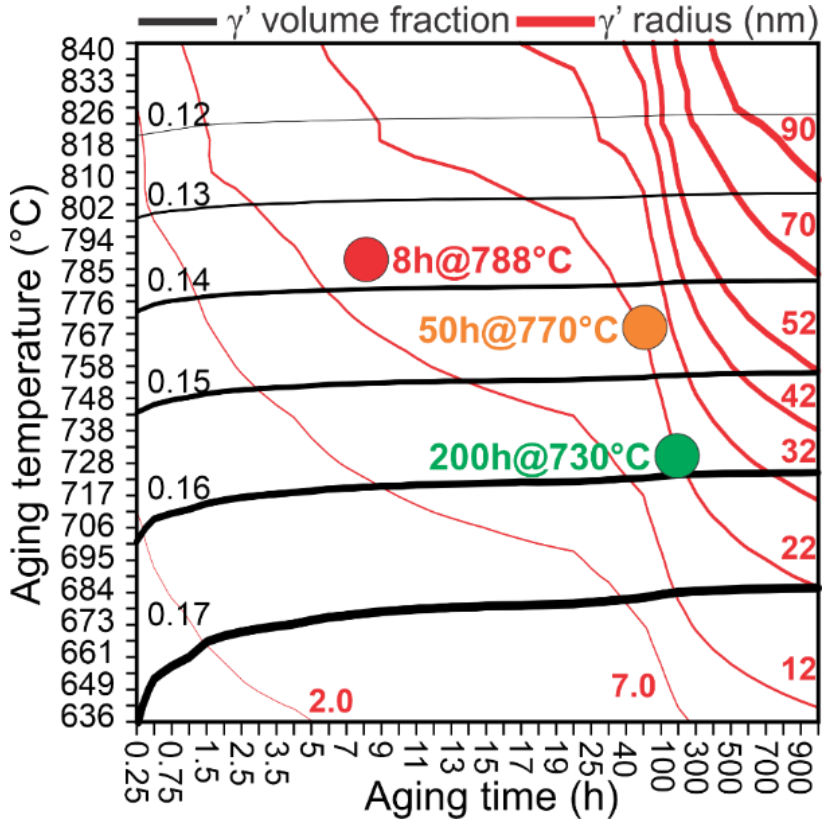


Xin Wang, Luis Fernando Ladinos Pizano, Soumya Sridar, Chantal Sudbrack, Wei Xiong, ***Science and Technology of Advanced Materials***, 25(1) (2024) 2346067. DOI: 10.1080/14686996.2024.2346067

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%.

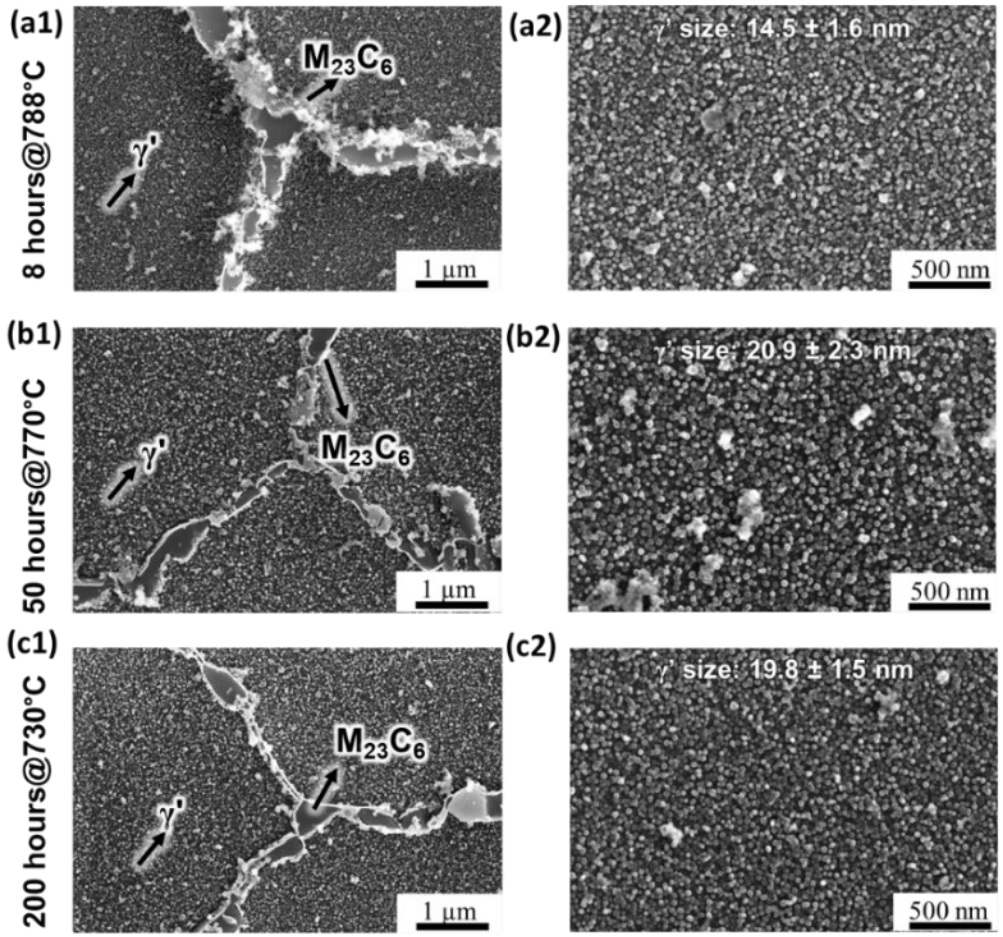


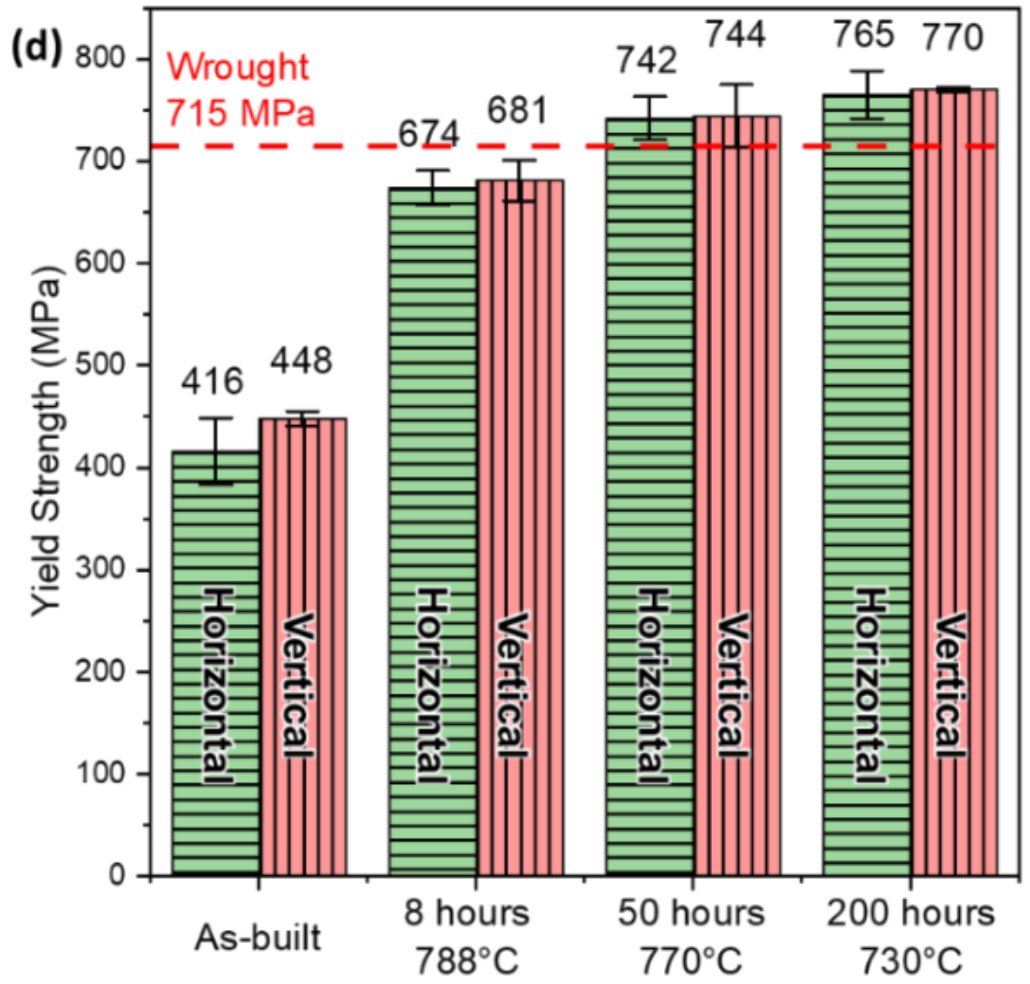


Xin Wang, Luis Fernando Ladinos Pizano, Soumya Sridar, Chantal Sudbrack, Wei Xiong, ***Science and Technology of Advanced Materials***, 25(1) (2024) 2346067.
DOI: 10.1080/14686996.2024.2346067

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 step aging





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Thank You for Your Attention! ☺

Physical Metallurgy and Materials Design Laboratory

Bridge Scientific Fundamentals and Engineering Applications

