High-Throughput Exploration of Refractory Superalloys with Experimental Verification

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Thermo-Calc Webinar

05/02/2024

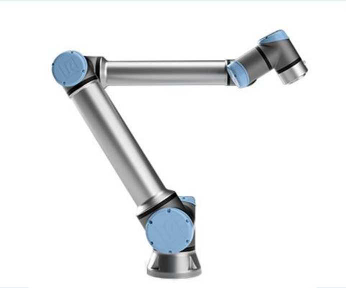
Kube Lab at UW-Madison

WISCONSIN
UNIVERSITY OF WISCONSIN–MADISON

Design and Physics of Complex Alloys

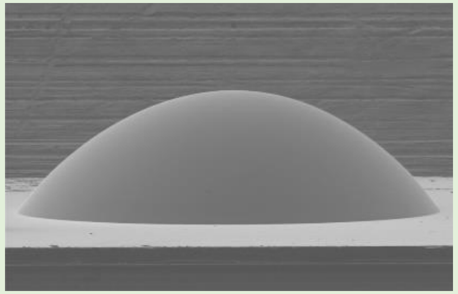
Pushing the Throughput Limit

- Accelerated synthesis and testing
- Combinatorial sputtering
- Rapid bulk synthesis



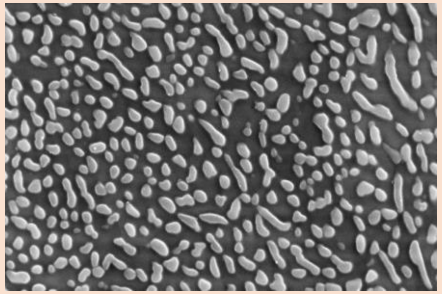
Pushing the Characterization Limit

- Metallic liquids: Structure and Viscosity
- Glass forming ability and glass transition
- Plasticity, strength, toughness…



Pushing the Performance Limit

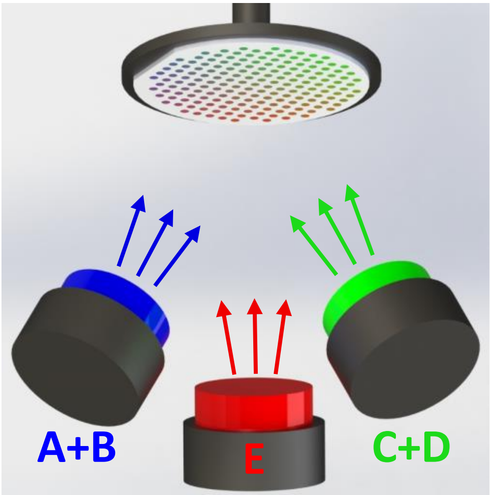
- Refractory Alloys: High *T*, Irradiation
- Designing new practical BMGs
- Thermal processing, Rapid solidification

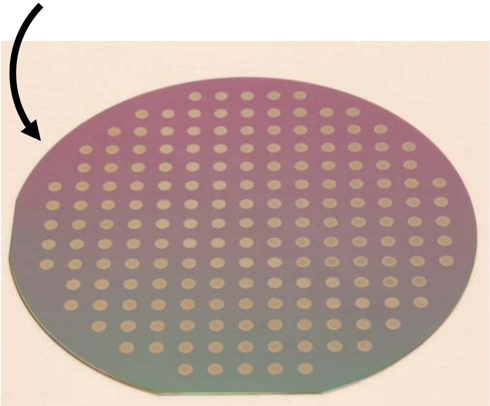


Thermo-Calc Software

1. Pushing the Throughput Limit:
Combinatorial sputtering for rapid phase mapping

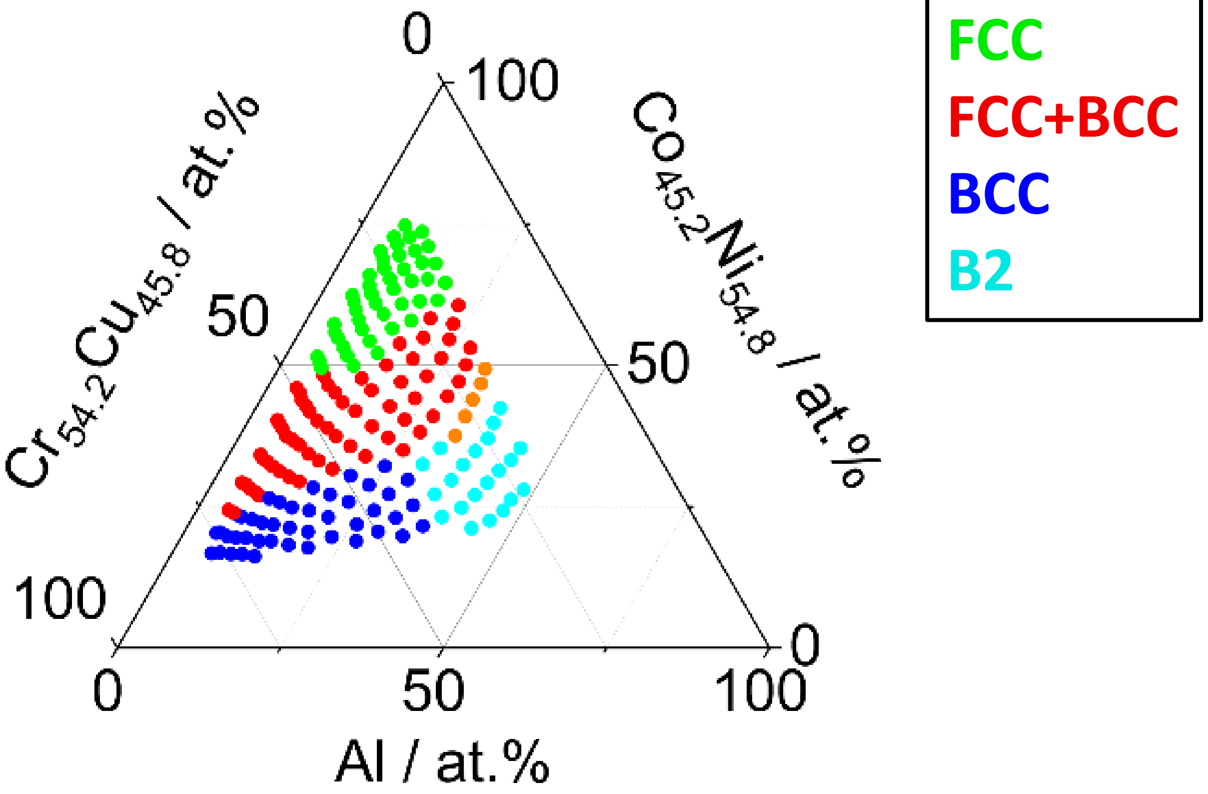
Co-Sputtering: 10^{10} K/sec





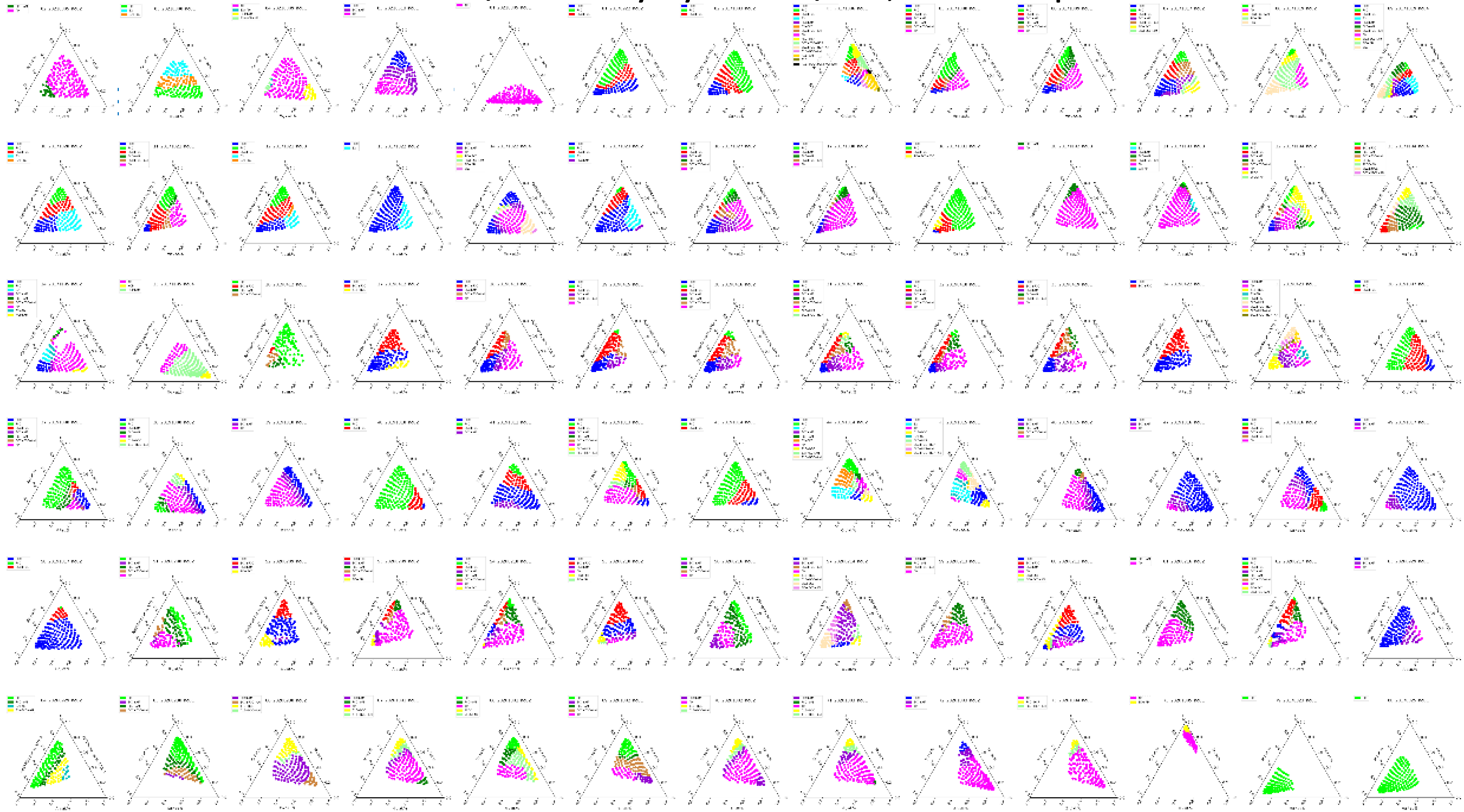
Automatic EDX and XRD →

Metastable phase map:



S.A. Kube, J. Schroers et al. / Acta Materialia 166 (2019) 677−686: *Phase Selection Motifs in High Entropy Alloys*
S.A. Kube and J. Schroers / Scripta Materialia 186 (2020) 392–400: *Metastability in High Entropy Alloys*

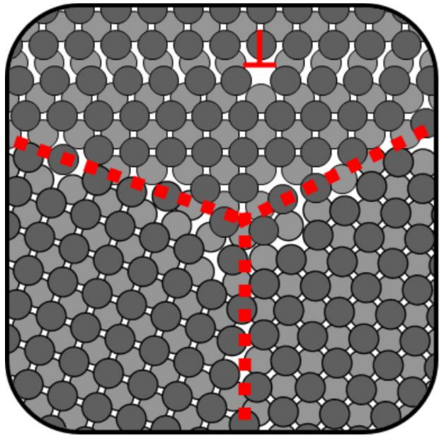
20 elements / 78 alloy systems / 13,500 compositions



2. Pushing the Characterization Limit:
What governs Metallic Glass forming ability?

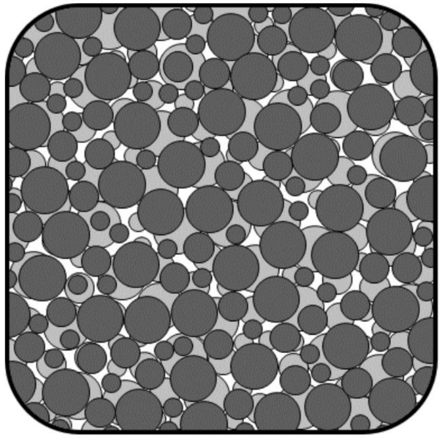
Slow cooling from melt: ⟷ Fast cooling from melt:

Polycrystal



ordered lattice,
grain boundaries,
dislocations

Glass



disordered,
continuous phase

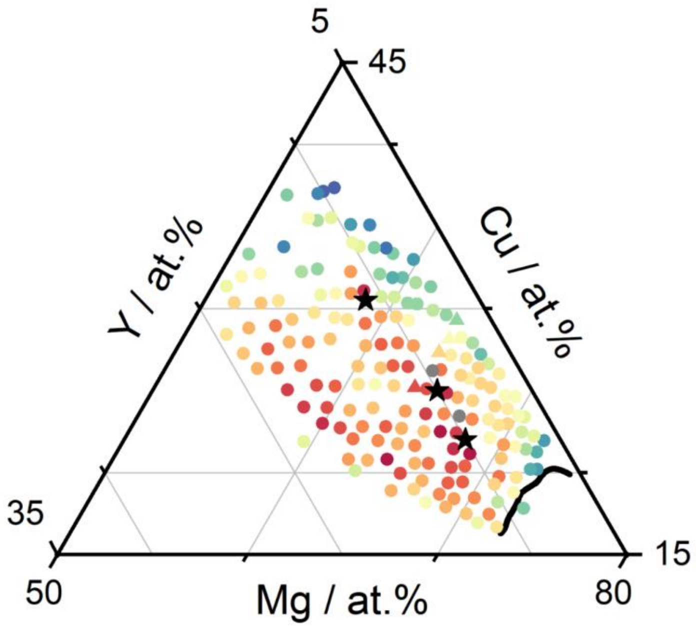
S.A. Kube, T. Pollock et al. (2024, under review):
Non-destructive evaluation of BMG components using RUS

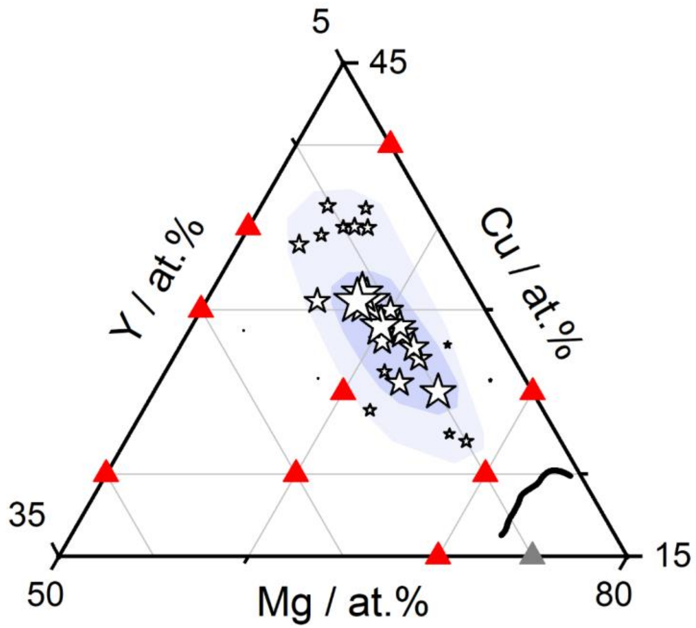
2. Pushing the Characterization Limit: What governs Metallic Glass forming ability?

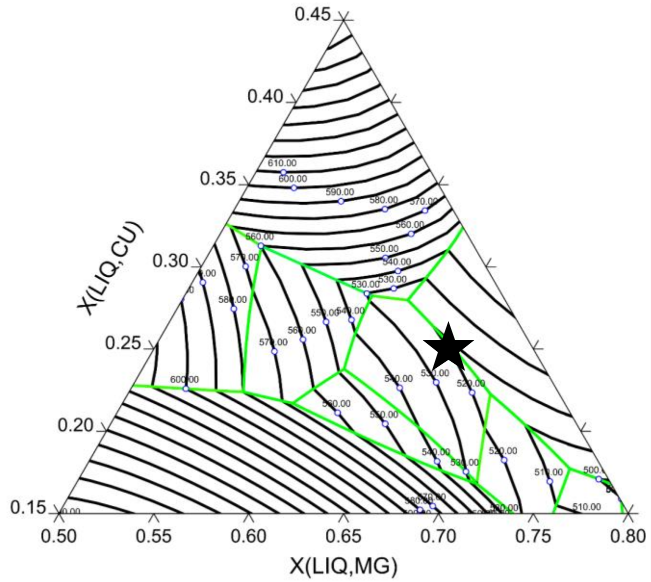
Kinetics? → **Glass Forming Ability** ← **Thermodynamics?**

E.g. Viscosity(T)

E.g. Liquidus projection







New "Film Inflation Method" (FIM)

Thermo-Calc Software

S.A. Kube, J. Schroers et al. / Nature Communications 13, 3708 (2022): Compositional dependence of the fragility in metallic glass forming liquids

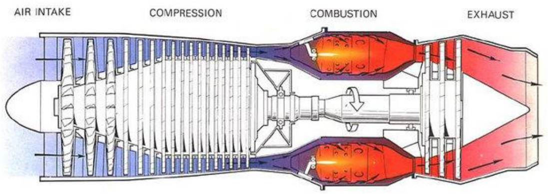
3. Pushing the Performance Limit: High-Throughput Exploration of Refractory Superalloys

Alloys for high temperatures and beyond

energy & sustainability, aerospace & defense

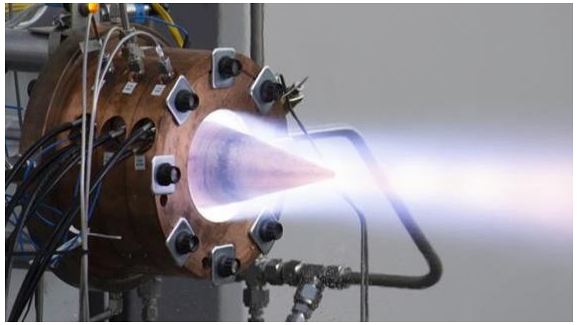
jet engines

‘Super’ superalloys: hotter, stronger, for even longer
University of Cambridge (2008)



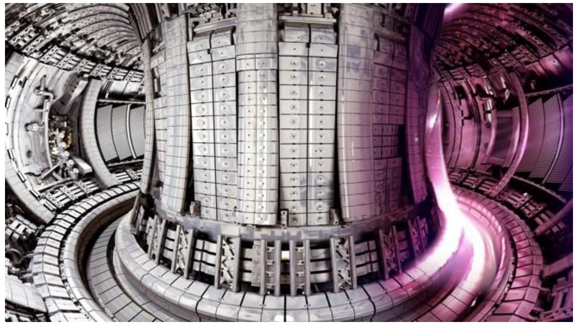
gas turbines

The Jet Engine, The Technical Publications Department, Rolls-Royce (1996)



rotating detonation engines

Rocket Shop℠ Defense Advanced Programs
Aerojet Rocketdyne (2023)



nuclear fusion

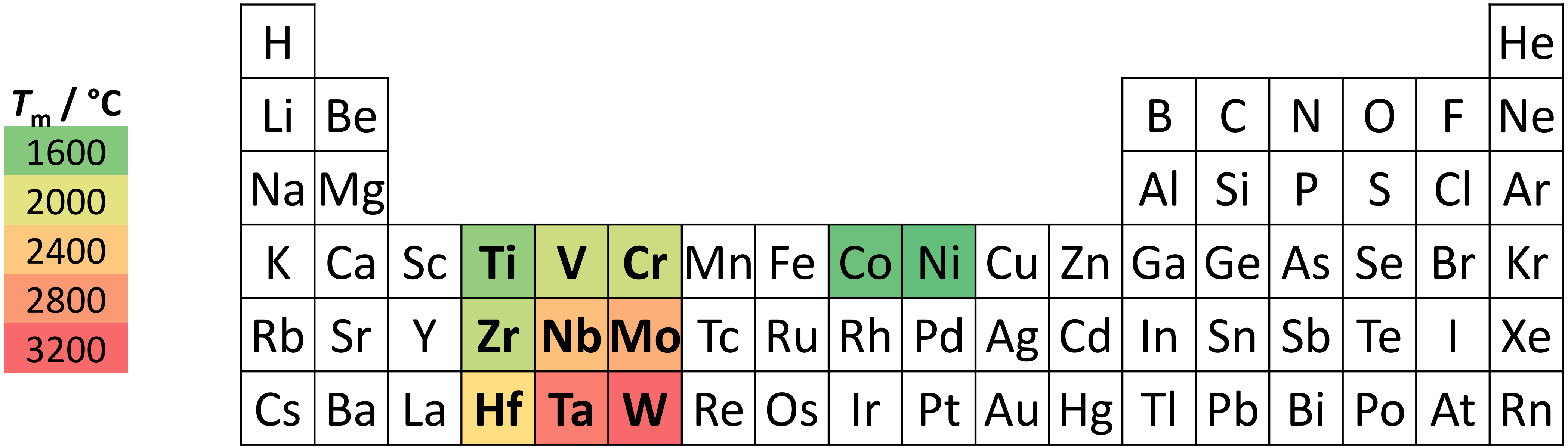
AJ Knowles, *Materials for fusion reactors*, Open Access Government (2023), *credit UKAEA*

Ni-superalloys: ≤ 1100°C
turbine operation > 1500°C

Now need: ≥ 1300°C
phase stability
thermal processability

also...
ductility, strength
creep, fatigue resistance
density, cost, manufacturability
oxidation resistance
irradiation tolerance

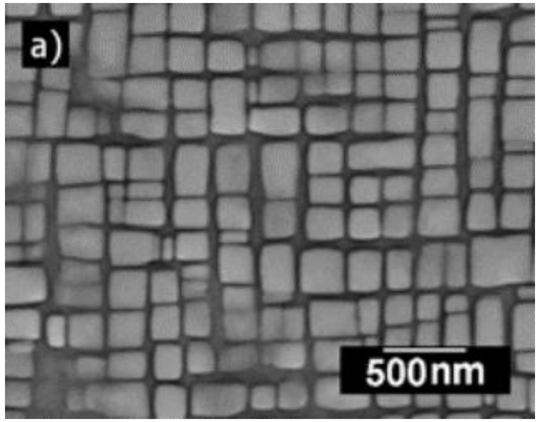
Refractory elements: High melting temperatures



“Refractory Superalloys”

Ni Superalloys

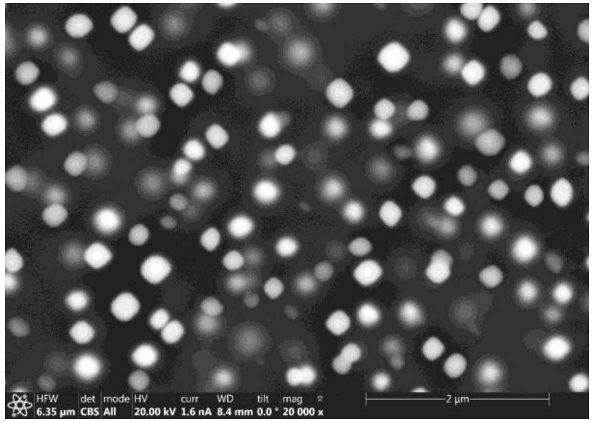
γ-FCC matrix, γ’-$L1_2$ precipitates



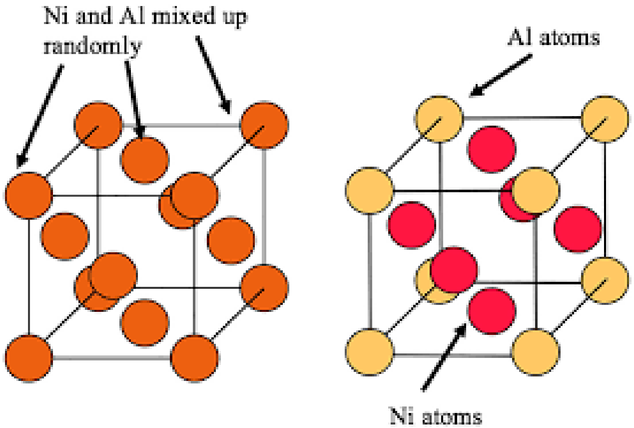
A. Bauer et al. *Superalloys 2012: 12th intl symp on Superalloys.*

“BCC-B2 microstructure”

BCC matrix, B2 precipitates

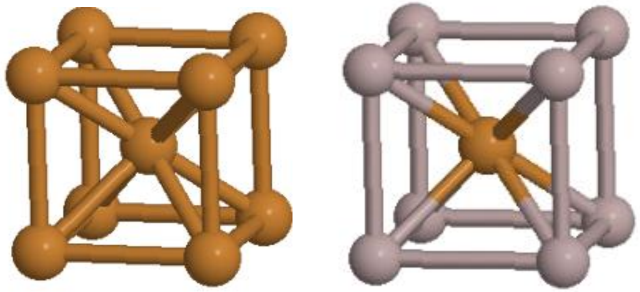


FCC



$L1_2$

BCC



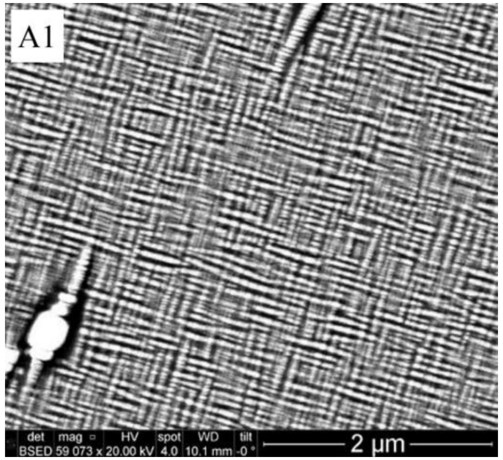
B2

Example 1: BCC + (Al,Ti,Zr) B2

$AlMo_{0.5}NbTa_{0.5}TiZr$
(24h at 1400°C,
Cooled 10 K/min here)

BCC (Nb rich)
B2 (Zr rich)

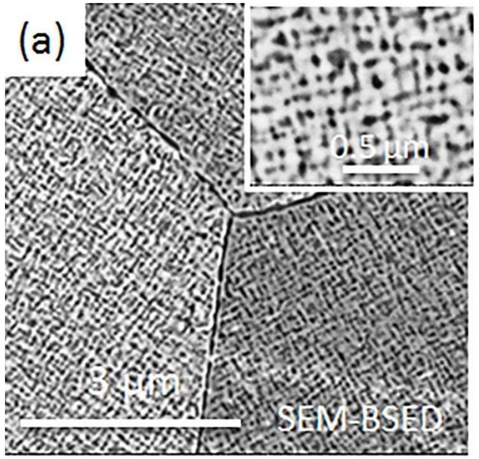
O. Senkov O, *et al.*
JOM 66, 2030–2042 (2014).

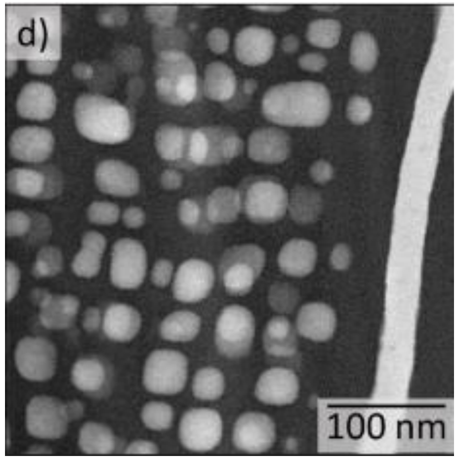


$Al_{0.5}$ Nb $Ta_{0.8}$ $Ti_{1.5}$ $V_{0.2}$ Zr
(120 h at 600°C here)

Matrix: BCC (Ti,NbTa,V)
Precipitates: B2 (Zr,Al,Ti)

V. Soni, R. Banerjee, *et al.*
Sci. Rep. 8, 1–10 (2018).





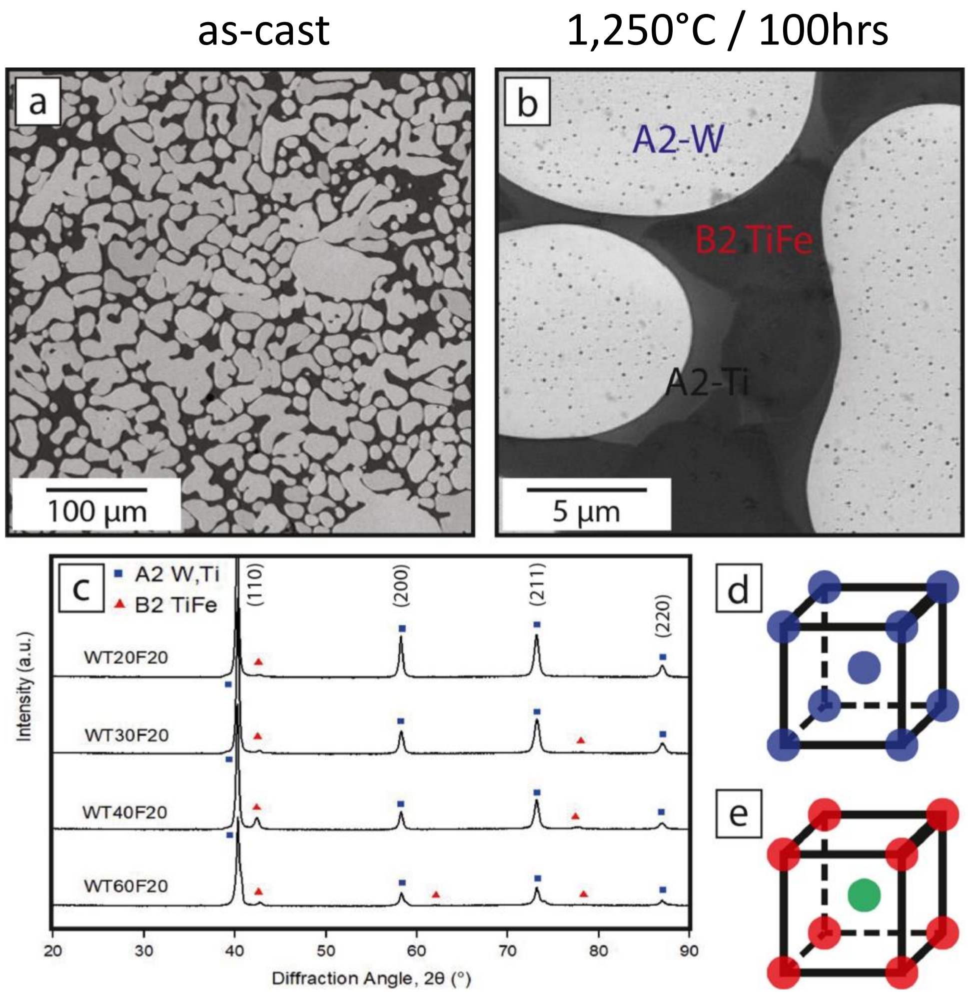
$Al_{0.5}$ Mo Ta Ti
(100 h at 1000°C here)

Matrix: B2 (Al,Ti)
Precipitates: BCC (Mo,Ta)

D. Schliephake, *et al.*
Scr. Mater. 173, 16–20 (2019).

Often inverted: B2 matrix, BCC precipitates
(Al,Ti,Zr) B2 not stable > 1200°C

Example 2: Ti_{30} Fe_{20} – W_{50}



W BCC dendrites
TiFe interdendritic B2 phase

- TiFe B2 melts at ~1340°C
- Homogenize W dendrites difficult
- Coherence difficult

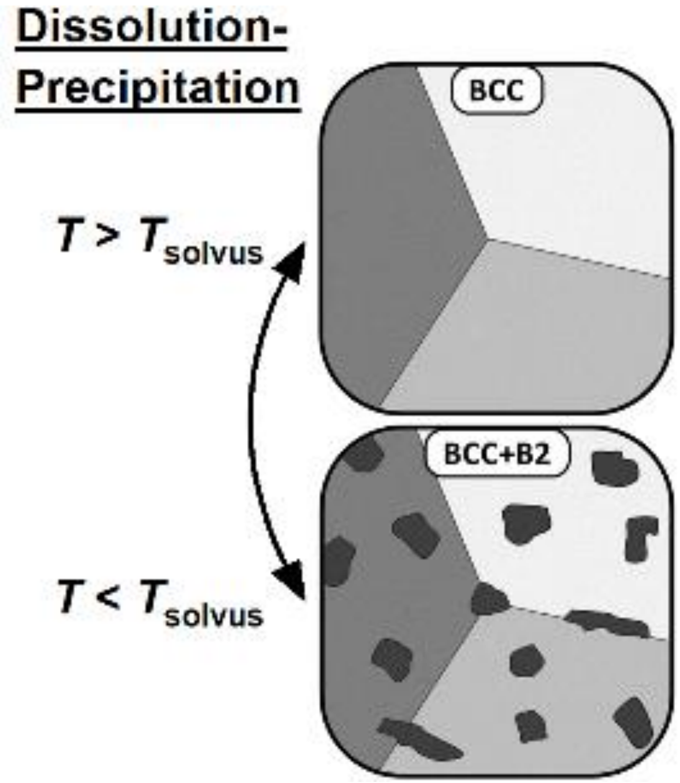
A.Knowles, et al., *Tungsten-based bcc-superalloys Applied Materials Today,* 23, 101014 (2021)

Our design goals

1. Phase stability:
   BCC matrix, B2 precipitates, stable ≥ 1300°C

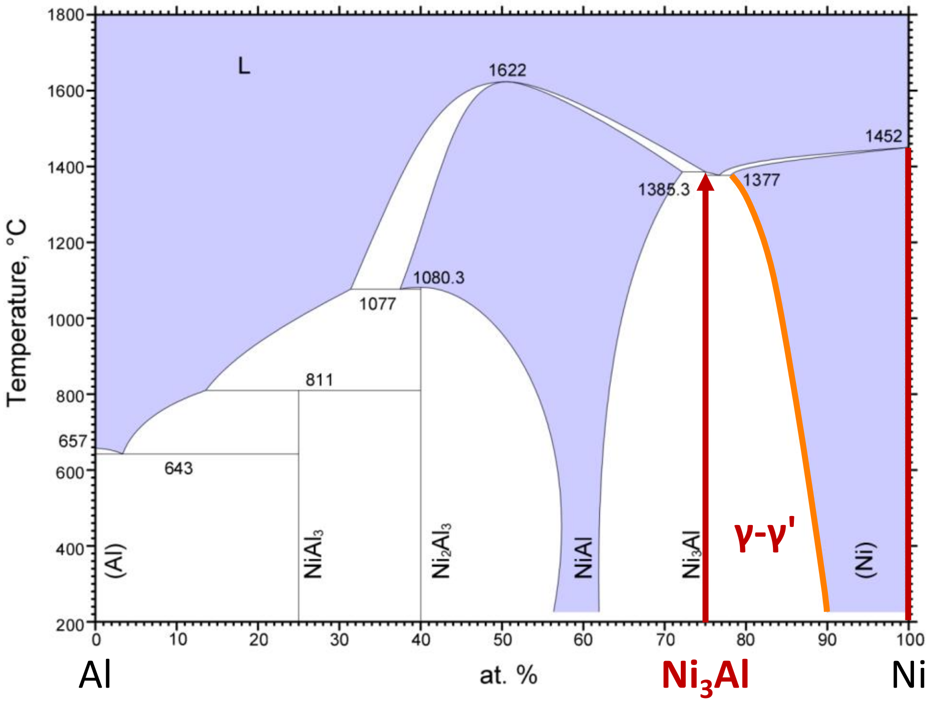
2. Thermal processability:
   Dissolution-precipitation pathway

3. Morphology:
   coherent, cuboidal, sub-micron particles



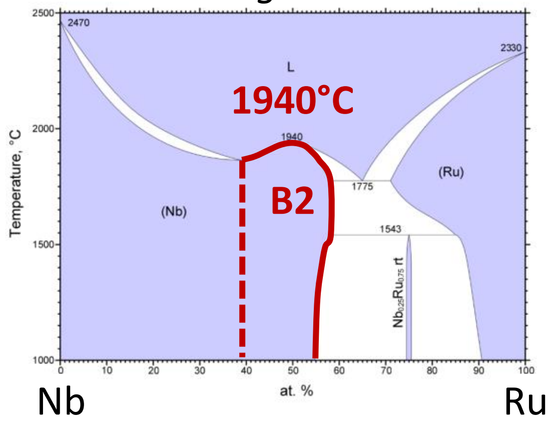
Binary BCC-B2 system?

Superalloys:
Ni-Al binary

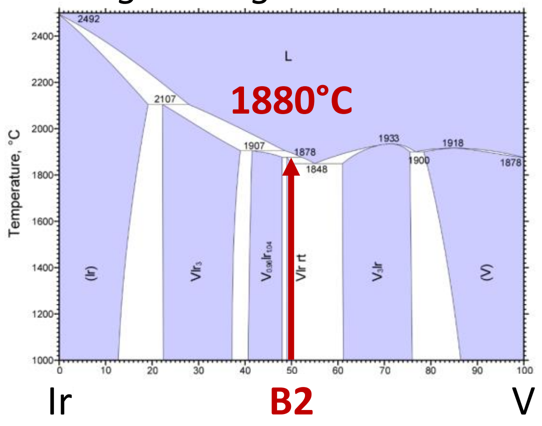


Refractory alloys:
10 known binaries with refractory element and stable B2 formation: none suitable

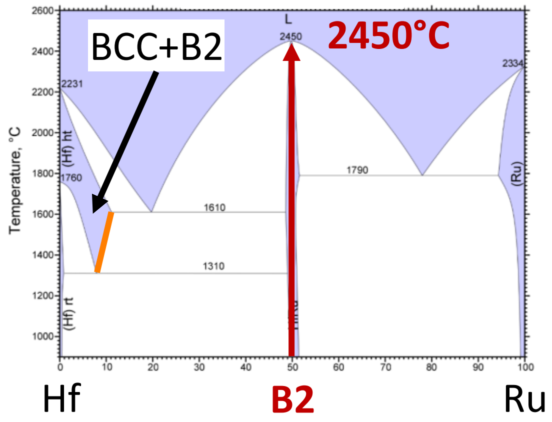
ordering transition



neighboring intermetallics



HCP element



Design strategy: Pseudobinary systems

a) 24 practical B2s: stability limit in °C

≥ 1750°C		≥ 1300°C		< 1300°C	
Ru - Hf	2450	Co - Hf	1740	Cu - Zr	940
Ru - Zr	2131	Co - Al	1640	Cu - Y	935
Ru - Ti	2120	Ni - Al	1639	Co - Fe	730
Ru - Al	2069	Co - Zr	1400	Re - Ti	?
Ru - Ta	2050	Co - Ti	1382	Re - Al	?
Ru - Nb	1942	Fe - Ti	1340	Fe - V	?
Ru - V	1800	Fe - Al	1310	Cu - Ti	?
		Ni - Ti	1307	Al - Ti	?
				Al - Y	?

b) Refractory BCC elements

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	**V**	**Cr**	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	**Nb**	**Mo**	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	**Ta**	**W**	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn

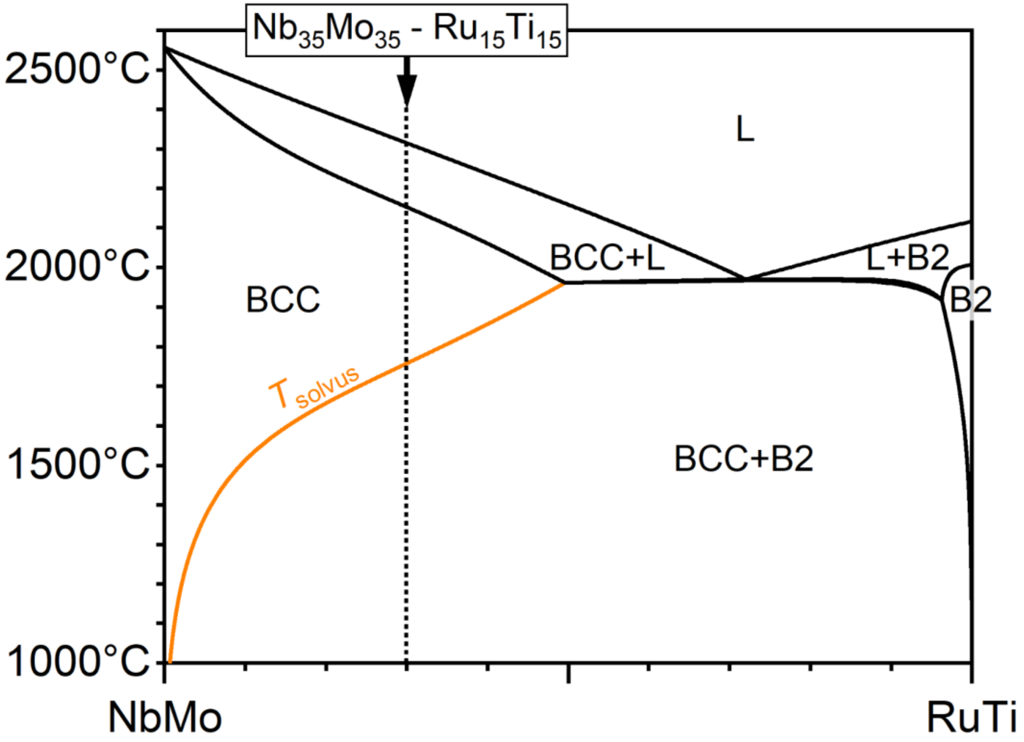
(Total of 279 B2 pairs in ICSD, mostly impractical elements.)

Example: RuTi (B2) + NbMo (BCC)

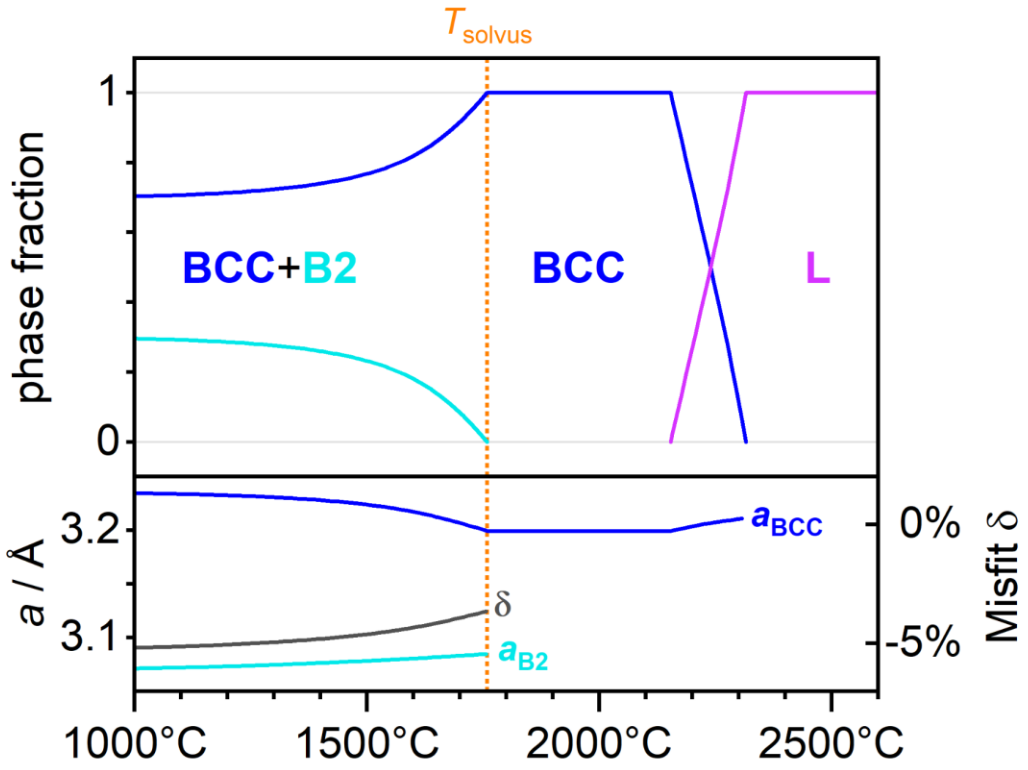
S. Kube, T. Pollock et al., Acta Mat. 265, 119628, (2024).

Example: RuTi B2 + NbMo BCC

a) Pseudobinary BCC-B2 phasediagram:



b) *T*-axis for $Nb_{35}Mo_{35}$ - $Ru_{15}Ti_{15}$:

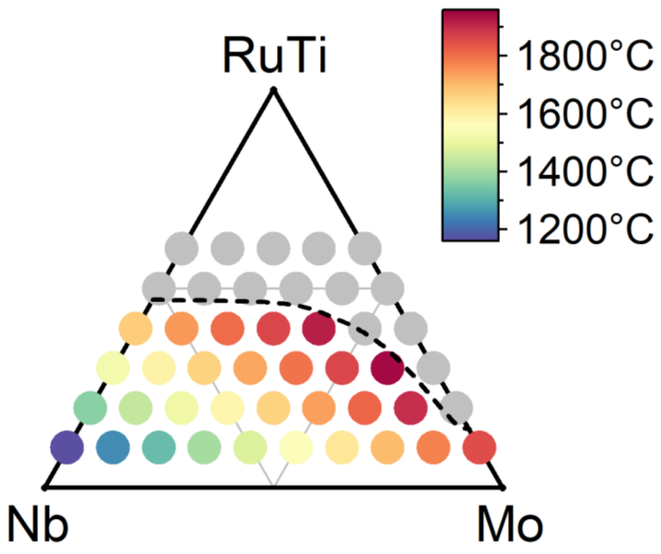


(calculated using TCHEA5 database)

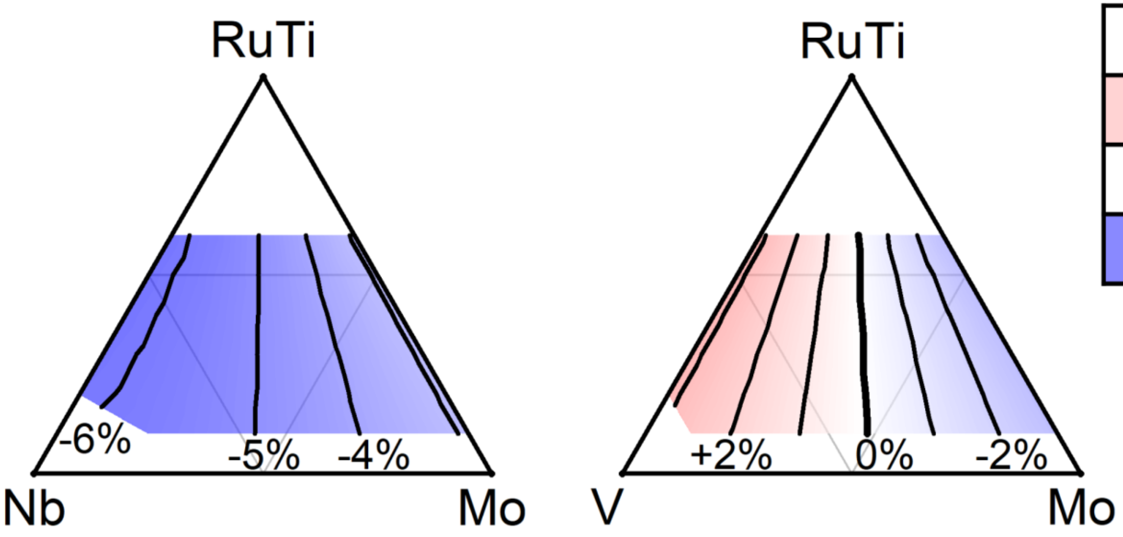
S. Kube, T. Pollock et al., Acta Mat. 265, 119628, (2024).

Microstructure optimization by composition

c) Solvus temperature:



d) Misfit at 1300°C, and lattice constants:



a_{B2} / Å		a_{BCC} / Å	
Ru-Al	3.01	V	2.97
Ru-Ti	3.07		
Ru-Hf	3.24	Mo	3.16
		W	3.18
		Nb	3.32
		Ta	3.32

(calculated using ThermoCalc / TCHEA5)

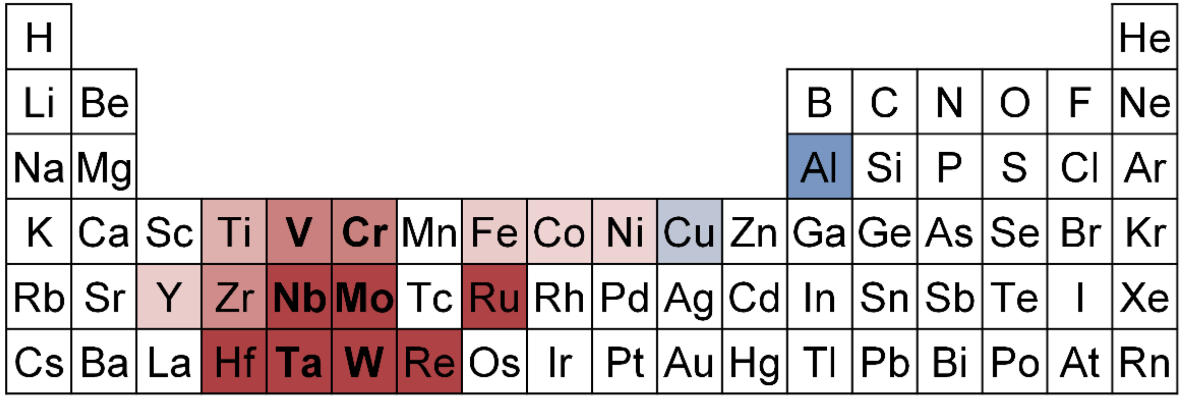
S. Kube, T. Pollock et al., Acta Mat. 265, 119628, (2024).

Numerous potential combinations

a) 24 practical B2s: stability limit in °C

≥ 1750°C		≥ 1300°C		< 1300°C	
Ru - Hf	2450	Co - Hf	1740	Cu - Zr	940
Ru - Zr	2131	Co - Al	1640	Cu - Y	935
Ru - Ti	2120	Ni - Al	1639	Co - Fe	730
Ru - Al	2069	Co - Zr	1400	Re - Ti	?
Ru - Ta	2050	Co - Ti	1382	Re - Al	?
Ru - Nb	1942	Fe - Ti	1340	Fe - V	?
Ru - V	1800	Fe - Al	1310	Cu - Ti	?
		Ni - Ti	1307	Al - Ti	?
				Al - Y	?

b) Potential matrix elements:



24 B2s x 153 matrix combinations (one or two elements) ≈ 3500 potential systems

S. Kube, T. Pollock et al., Acta Mat. 265, 119628, (2024).

Thermo-Calc – Python: High-throughput search

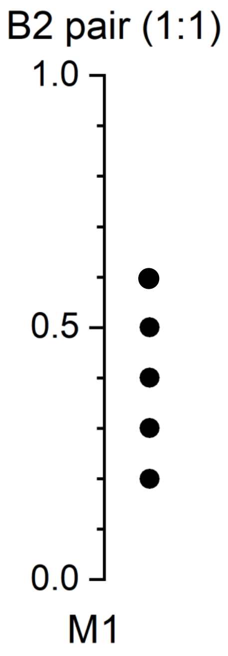
1) Generate ternaries and quaternaries:

$B_1\ B_2 - M_1$ and $B_1\ B_2 - M_1\ M_2$

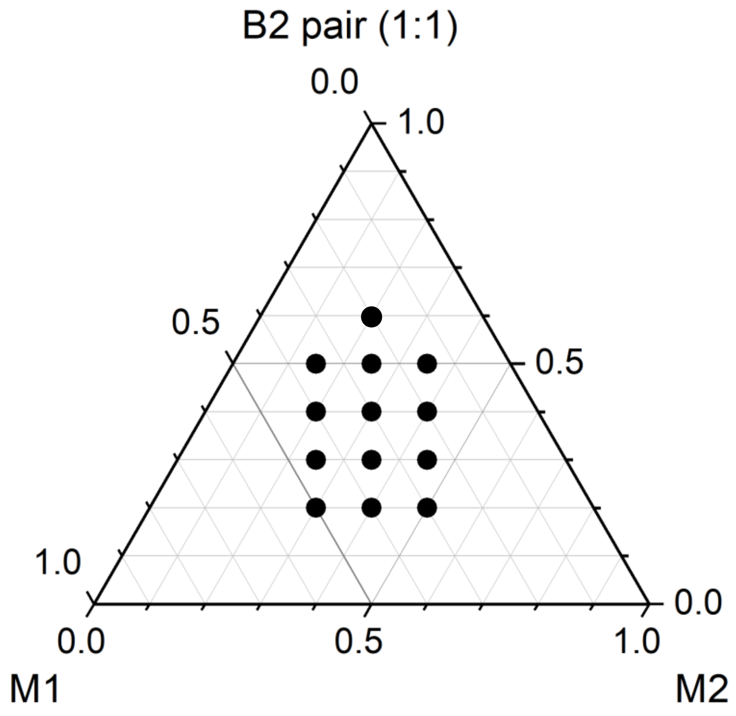
	Arity	B2_1	B2_2	Mat_1	Mat_2
0	3	Al	Ru	Nb	
1	3	Al	Ru	Ta	
2	3	Nb	Ru	Ta	
3	3	Ru	Ta	Nb	
			…		
58	4	Al	Ru	Nb	Ta
59	4	Al	Ru	Ti	Nb
60	4	Al	Ru	Ti	Ta
61	4	Ti	Ru	Nb	Ta
			…		

Σ 3500 systems

2) Test multiple compositions in each system:



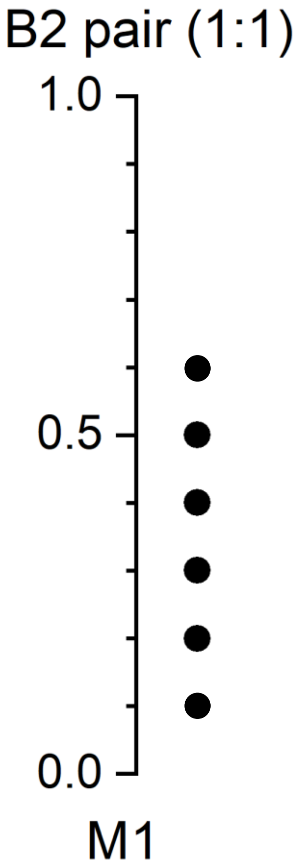
Ternary



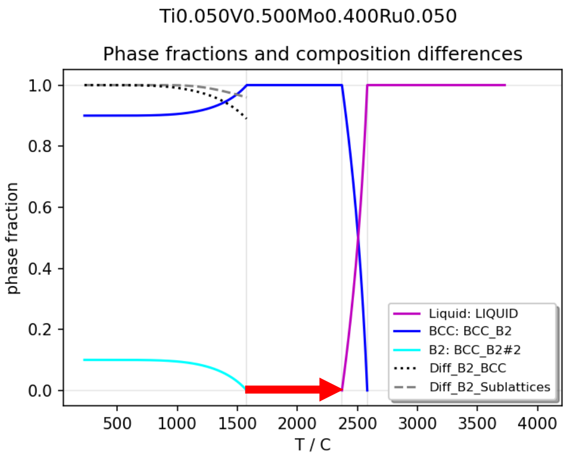
Quaternary

S. Kube, T. Pollock et al., Acta Mat. 265, 119628, (2024).

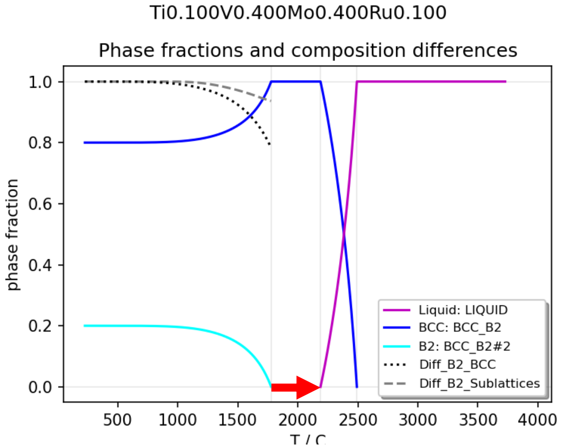
Thermo-Calc – Python: High-throughput search



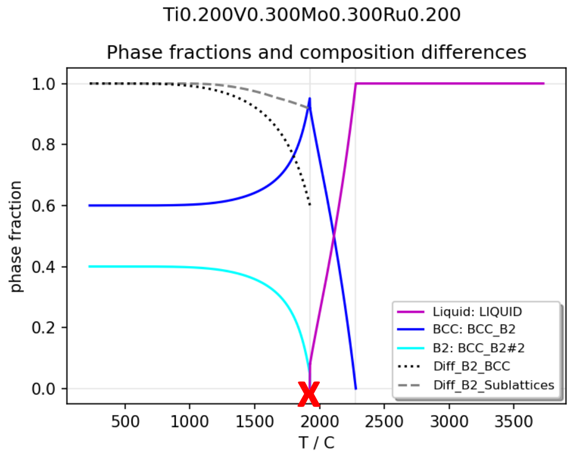
10% B2



20% B2



40% B2

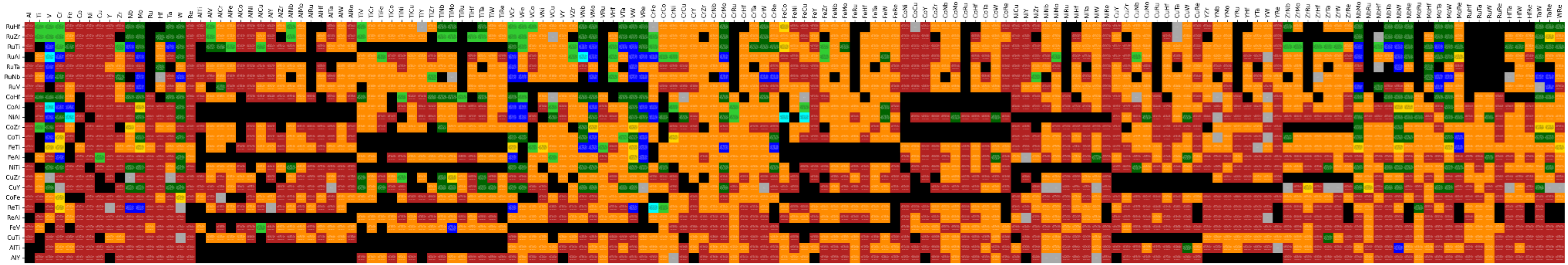


Ru Ti – V Mo

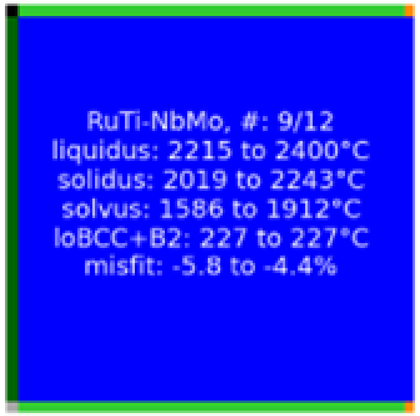
S. Kube, T. Pollock et al., Acta Mat. 265, 119628, (2024).

Map of BCC-B2 alloy systems

24 B2s x 153 matrix element combinations



field close-up:



* high-res map in our SI here:
"Navigating the BCC-B2 refractory alloy space"

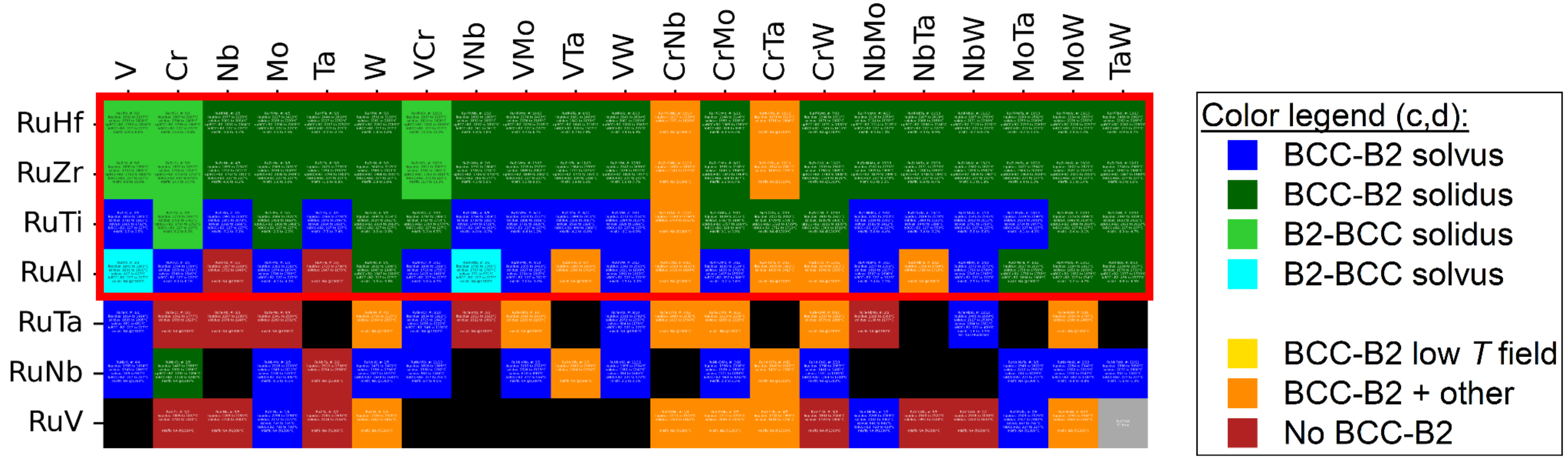
Color legend (c,d):
- BCC-B2 solvus
- BCC-B2 solidus
- B2-BCC solidus
- B2-BCC solvus
- BCC-B2 low *T* field
- BCC-B2 + other
- No BCC-B2

(calculated using ThermoCalc-Python / TCHEA5)

S. Kube, T. Pollock et al., Acta Mat. 265, 119628, (2024).

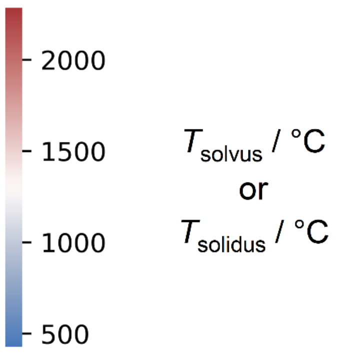
Ru-B2 RMPEA space

d) Reduced space: Ru-B2s x Refractory BCC elements



e) Reduced space: BCC-B2 stability limit in °C

	V	Cr	Nb	Mo	Ta	W	VCr	VNb	VMo	VTa	VW	CrNb	CrMo	CrTa	CrW	NbMo	NbTa	NbW	MoTa	MoW	TaW
RuHf	1824	1805	2004	2209	2252	2283	1828	1832	2185	2139	2163		1985		1970	2179	2188	2230	2269	2257	2285
RuZr	1805	1752	1811	2049	1903	2041	1801	1710	2002	1875	1977		1969		1888	1999	1893	1987	2028	2053	1988
RuTi	1732	1761	1666	1968	1930	2063	1774	1721	1920	1826	1896		1894	1729	1870	1912	1898	1793	1977	2034	2032
RuAl	427	1549		1786		1906	1461	571	1925		1813		1555			1696		1745	1758	1878	1733
RuTa	651						1222				1175							1501			
RuNb	957	1396		1453		1677	1484		896		1645		1496		1383				1029	1542	1501
RuV				754												981			765		



1. **RuHf, RuZr:**
   High stability, no solvus
2. **RuTi:**
   High stability, with solvus
3. **RuAl:**
   High stability, with solvus, but prone to intermetallics

CALPHAD:
Predict likely competing phases.
→ Good filter for negatives!

But:
What about predicted BCC-B2?
→ Experimental verification!

S. Kube, T. Pollock et al., Acta Mat. 265, 119628, (2024).

Experimental survey

<u>Select composition grid:</u>

B2: Select RuHf, RuTi, RuAl

BCC: Select V, Nb, Mo, Ta

Comp: $B1_{15}\ B2_{15} - M1_{70}$ or

$B1_{15}\ B2_{15} - M1_{35}\ M2_{35}$

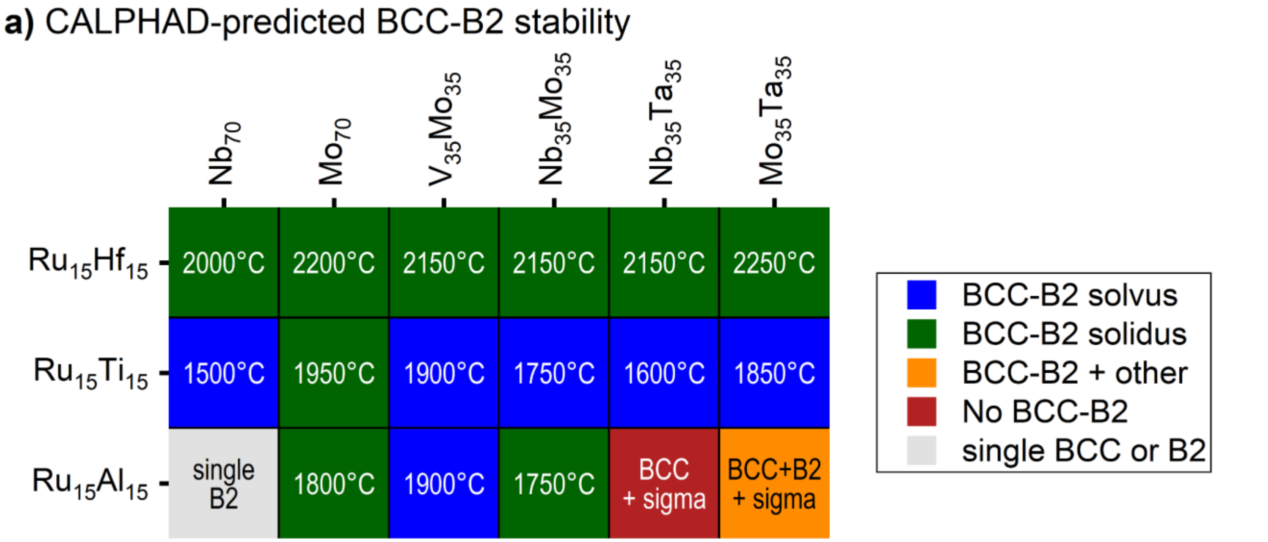
<u>Experimental procedure:</u>

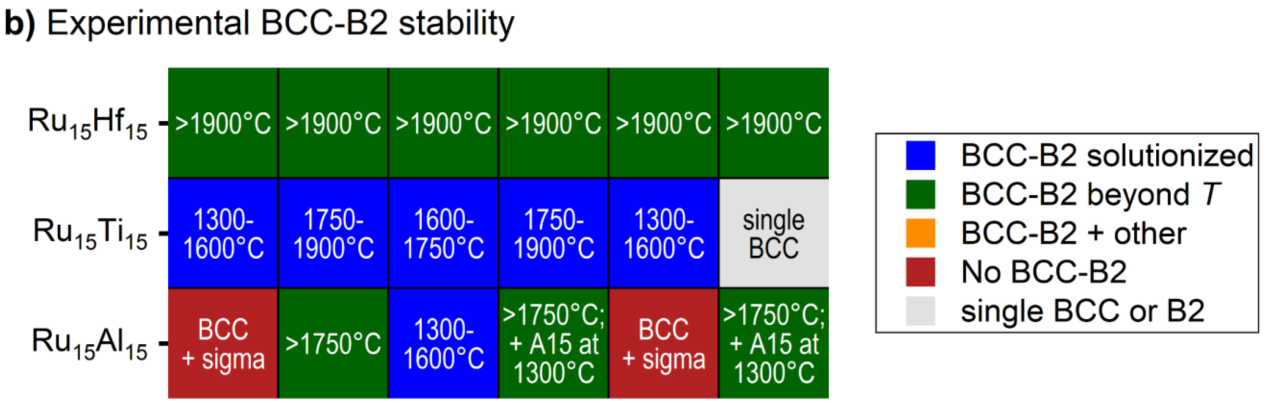
Arc melt:
- 18 compositions x 20g buttons

Anneal 1: (solutionize)
- 1750°C/10hrs
- 1900°C/10hrs

Anneal 2: (precipitate)
- 1600°C/40hrs
- 1300°C/200hrs

Characterize:
- XRD, SEM
- (microhardness, compression, TEM)



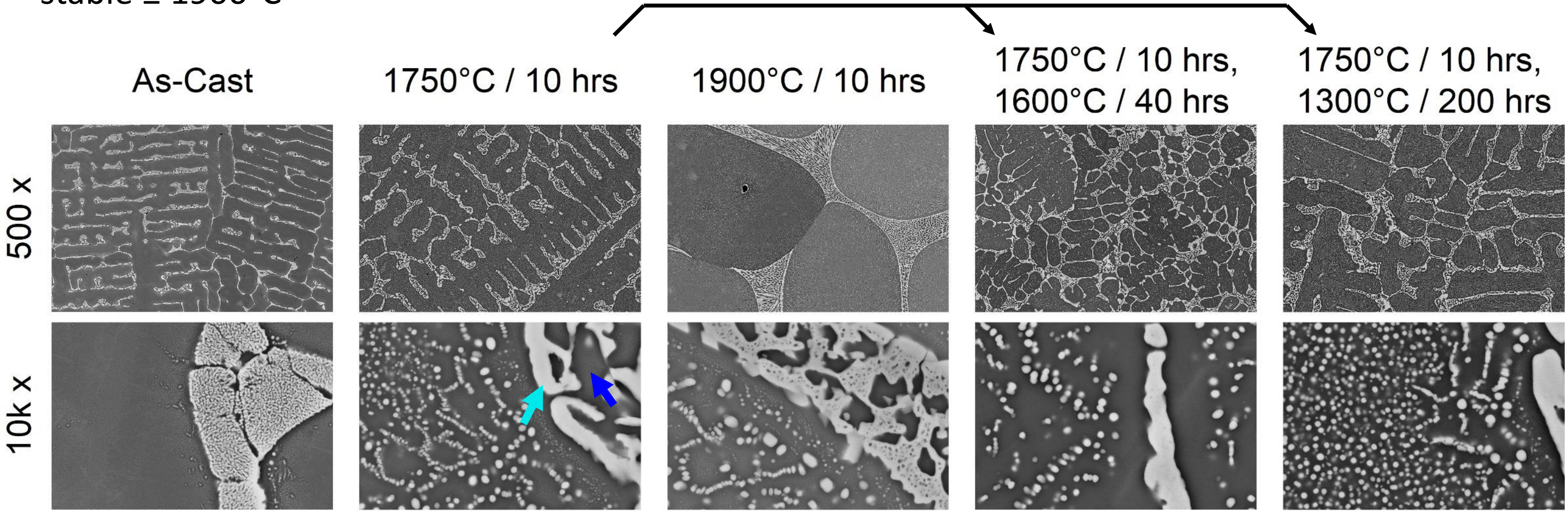


S. Kube, T. Pollock et al., Acta Mat. 265, 119628, (2024).

Example 1: $Ru_{15}\,Hf_{15} - Nb_{70}$

	Nb_{70}	Mo_{70}	$V_{35}Mo_{35}$	$Nb_{35}Mo_{35}$	$Nb_{35}Ta_{35}$	$Mo_{35}Ta_{35}$
$Ru_{15}Hf_{15}$	>1900°C	>1900°C	>1900°C	>1900°C	>1900°C	>1900°C
$Ru_{15}Ti_{15}$	1300-1600°C	1750-1900°C	1600-1750°C	1750-1900°C	1300-1600°C	single BCC
$Ru_{15}Al_{15}$	BCC + sigma	>1750°C	1300-1600°C	>1750°C; + A15 at 1300°C	BCC + sigma	>1750°C; + A15 at 1300°C

Nb BCC dendrites
RuHf B2 interdendritic
stable ≥ 1900°C



Scalebar: ▬▬▬ corresponds to 500x: 100μm | 5k x: 10μm | 10k x: 5μm

Example 2: Ru_{15} Ti_{15} – Nb_{70}

	Nb_{70}	Mo_{70}	$V_{35}Mo_{35}$	$Nb_{35}Mo_{35}$	$Nb_{35}Ta_{35}$	$Mo_{35}Ta_{35}$
$Ru_{15}Hf_{15}$	>1900°C	>1900°C	>1900°C	>1900°C	>1900°C	>1900°C
$Ru_{15}Ti_{15}$	1300-1600°C	1750-1900°C	1600-1750°C	1750-1900°C	1300-1600°C	single BCC
$Ru_{15}Al_{15}$	BCC + sigma	>1750°C	1300-1600°C	>1750°C; + A15 at 1300°C	BCC + sigma	>1750°C; + A15 at 1300°C

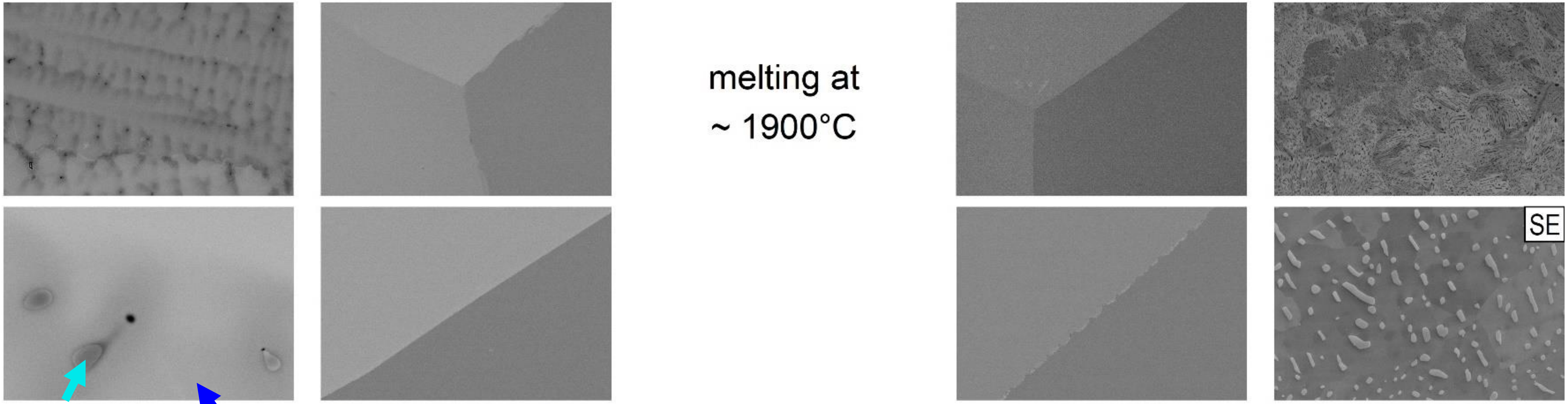
Nb BCC + RuTi B2

B2 dissolves between 1300 and 1600°C.

As-Cast	Homogenize & Solutionize		Precipitate & Age	
	1750°C / 10 hrs	1900°C / 10 hrs	1600°C / 40 hrs	1300°C / 200 hrs

500 x

5k x



11%, 0.5µm

Scalebar: ▬▬▬ corresponds to 500x: 100µm | 5k x: 10µm | 10k x: 5µm | 20k x: 2.5µm | 50k x: 1µm

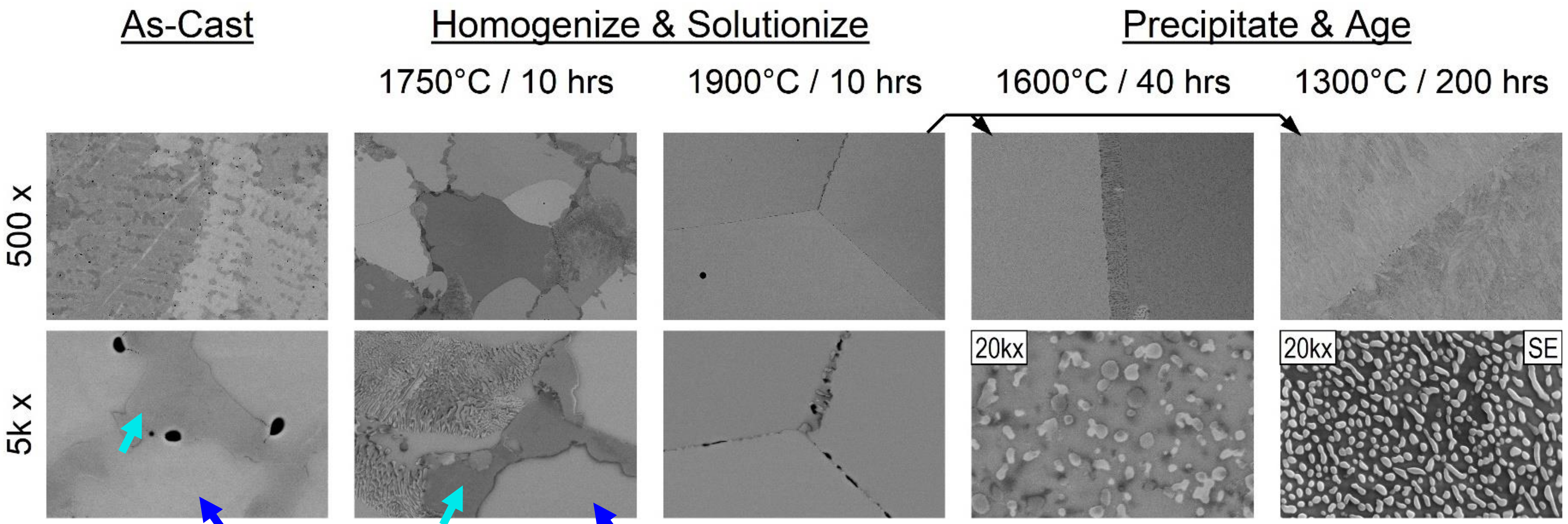
Example 3: Ru_{15} Ti_{15} – Nb_{35} Mo_{35}

	Nb_{70}	Mo_{70}	$V_{35}Mo_{35}$	$Nb_{35}Mo_{35}$	$Nb_{35}Ta_{35}$	$Mo_{35}Ta_{35}$
$Ru_{15}Hf_{15}$	>1900°C	>1900°C	>1900°C	>1900°C	>1900°C	>1900°C
$Ru_{15}Ti_{15}$	1300-1600°C	1750-1900°C	1600-1750°C	1750-1900°C	1300-1600°C	single BCC
$Ru_{15}Al_{15}$	BCC + sigma	>1750°C	1300-1600°C	>1750°C; + A15 at 1300°C	BCC + sigma	>1750°C; + A15 at 1300°C

NbMo BCC + RuTi B2

B2 dissolves between 1750 and 1900°C.

Misfit = −3.5%



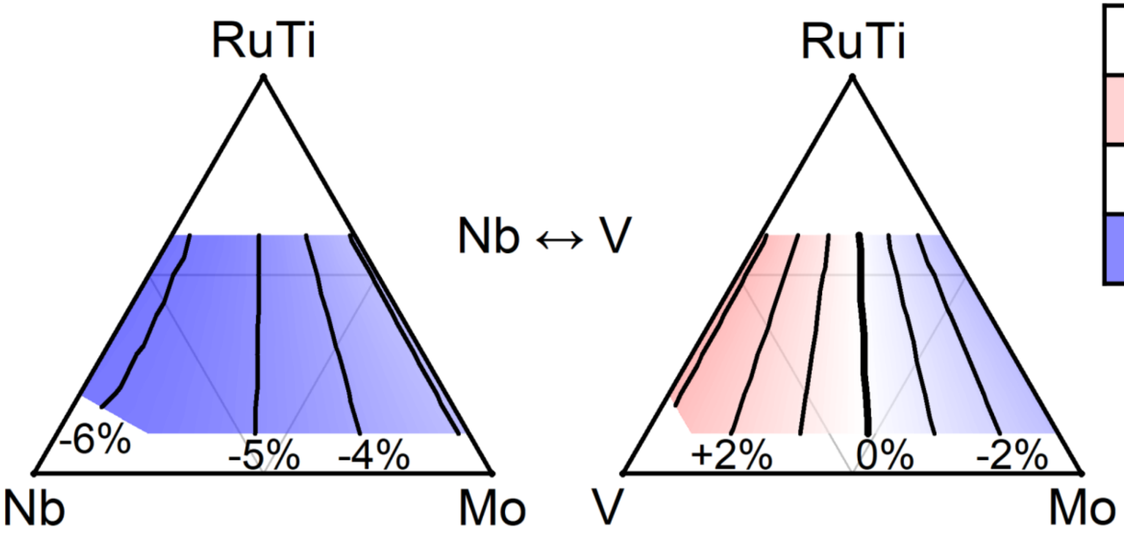
17%, 300 nm

24%, 125 nm

Scalebar: ▬ corresponds to 500x: 100µm | 5k x: 10µm | 10k x: 5µm | 20k x: 2.5µm | 50k x: 1µm

Reduce misfit by substitution

d) Misfit at 1300°C, and lattice constants:



a_{B2} / Å		a_{BCC} / Å	
Ru-Al	3.01	V	2.97
Ru-Ti	3.07		
Ru-Hf	3.24	Mo	3.16
		W	3.18
		Nb	3.32
		Ta	3.32

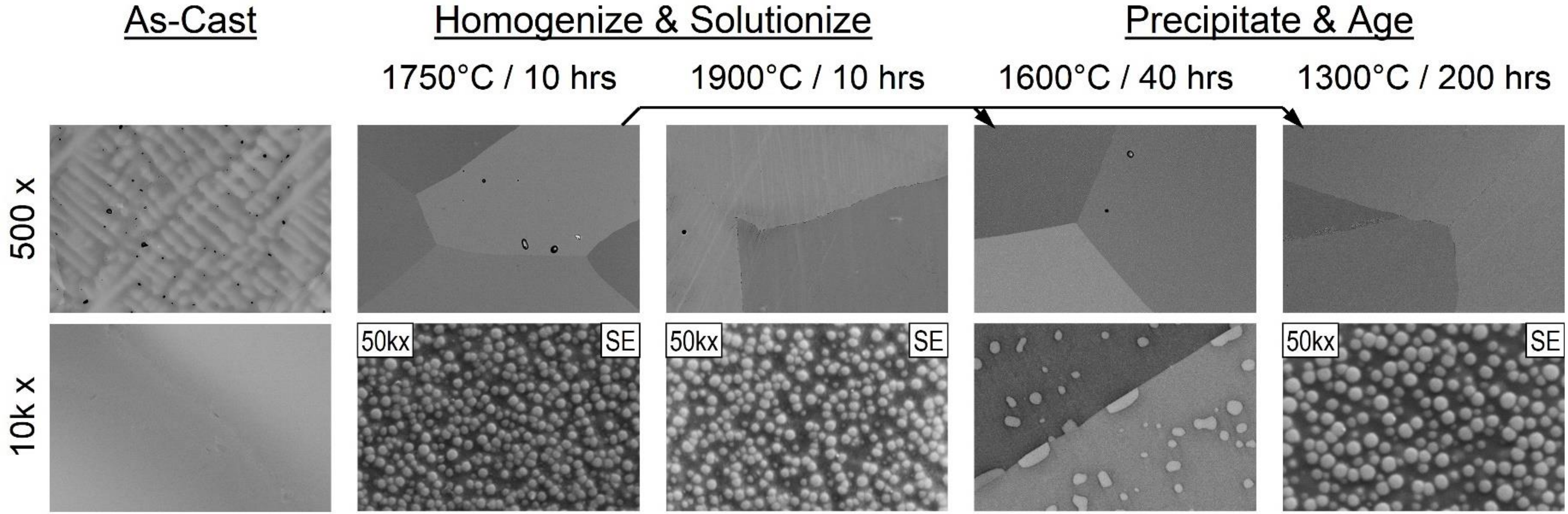
S. Kube, T. Pollock et al., Acta Mat. 265, 119628, (2024).

Example 4: $Ru_{15}\ Ti_{15} - V_{35}\ Mo_{35}$

VMo BCC + RuTi B2, stable ≥ 1600°C

B2 dissolves at 1750 and 1900°C, but precipitates on cooling.

	Nb_{70}	Mo_{70}	$V_{35}Mo_{35}$	$Nb_{35}Mo_{35}$	$Nb_{35}Ta_{35}$	$Mo_{35}Ta_{35}$
$Ru_{15}Hf_{15}$	>1900°C	>1900°C	>1900°C	>1900°C	>1900°C	>1900°C
$Ru_{15}Ti_{15}$	1300-1600°C	1750-1900°C	1600-1750°C	1750-1900°C	1300-1600°C	single BCC
$Ru_{15}Al_{15}$	BCC + sigma	>1750°C	1300-1600°C	>1750°C; + A15 at 1300°C	BCC + sigma	>1750°C; + A15 at 1300°C



70 nm particles | **70 nm** particles | coarsening to **400 nm** particles | minimal coarsening **90 nm** particles

Scalebar: ▬ corresponds to 500x: 100µm | 5k x: 10µm | 10k x: 5µm | 20k x: 2.5µm | 50k x: 1µm

Example 5: Ru_{15} Al_{15} – V_{35} Mo_{35}

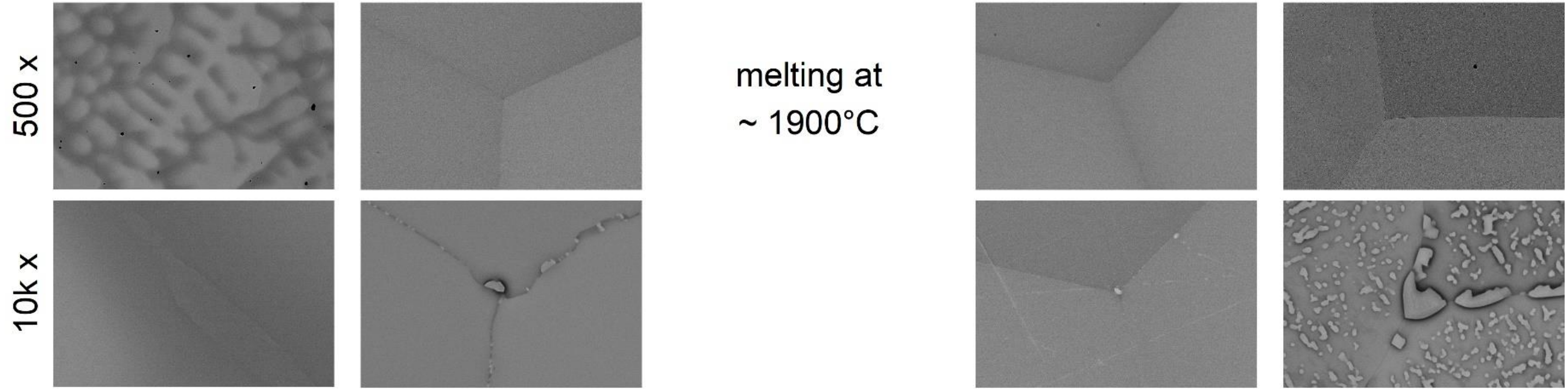
VMo BCC + RuAl B2

B2 dissolves between 1300 and 1600°C.

	Nb_{70}	Mo_{70}	$V_{35}Mo_{35}$	$Nb_{35}Mo_{35}$	$Nb_{35}Ta_{35}$	$Mo_{35}Ta_{35}$
$Ru_{15}Hf_{15}$	>1900°C	>1900°C	>1900°C	>1900°C	>1900°C	>1900°C
$Ru_{15}Ti_{15}$	1300-1600°C	1750-1900°C	1600-1750°C	1750-1900°C	1300-1600°C	single BCC
$Ru_{15}Al_{15}$	BCC + sigma	>1750°C	1300-1600°C	>1750°C; + A15 at 1300°C	BCC + sigma	>1750°C; + A15 at 1300°C

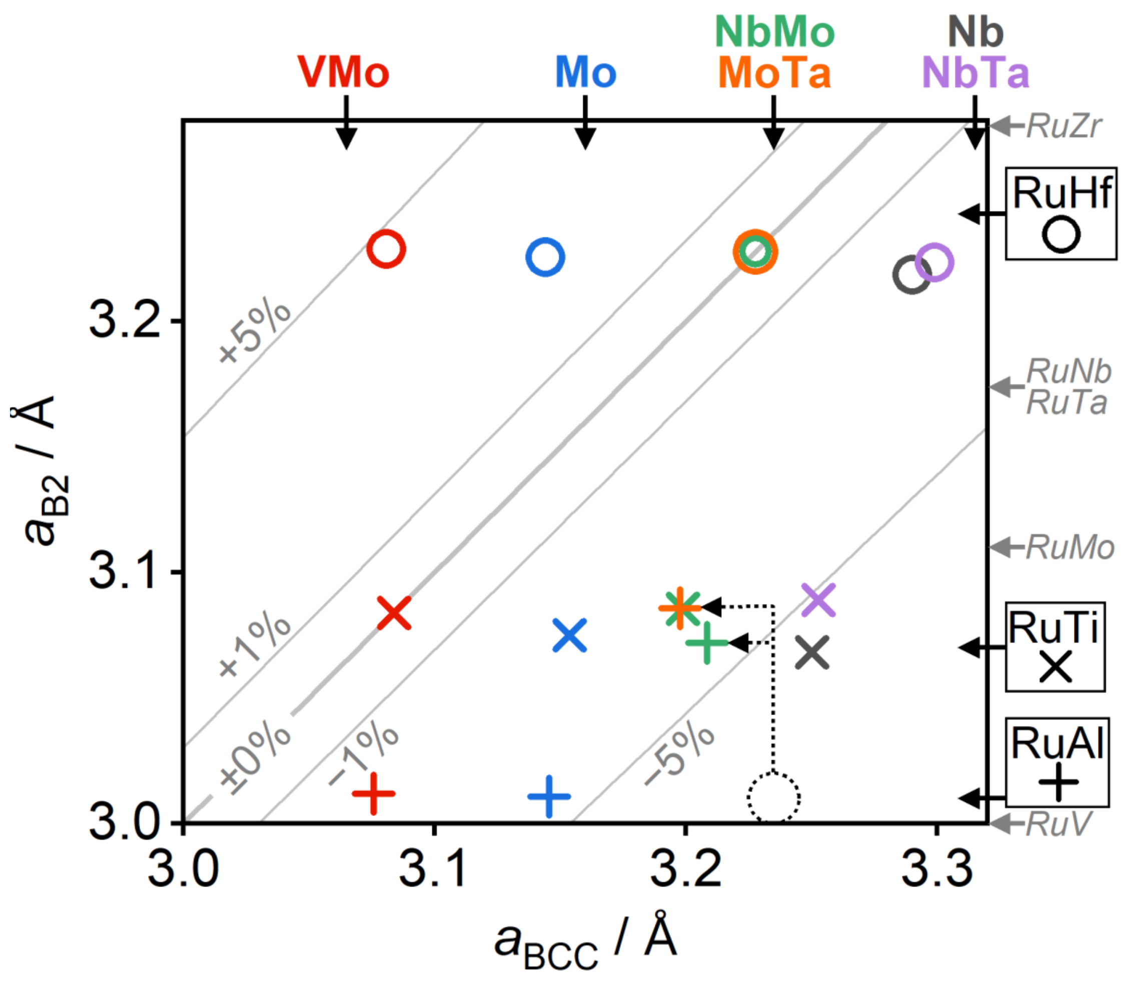
As-Cast | Homogenize & Solutionize | Precipitate & Age

1750°C / 10 hrs | 1900°C / 10 hrs | 1600°C / 40 hrs | 1300°C / 200 hrs



Scalebar: ——— corresponds to 500x: 100μm | 5k x: 10μm | 10k x: 5μm | 20k x: 2.5μm | 50k x: 1μm

Minimize misfit for coherence: Experimental from XRD



⊕ Best fit with Nb, Mo, Ta.
⊖ Limited processability.

⊖ Too small for Nb, Mo, Ta.
⊕ Best processability.

S. Kube, T. Pollock et al., Acta Mat. 265, 119628, (2024).

Conclusions

1. **RuHf B2:**
   exceptionally stable beyond 1900°C, no dissolution.
2. **RuTi B2:**
   stable up to 1900°C, dissolution between 1300 and 1900°C
3. **RuAl B2:**
   stable up to 1750°C, dissolution between 1300 and 1600°C
   prone to intermetallics with Nb and Ta

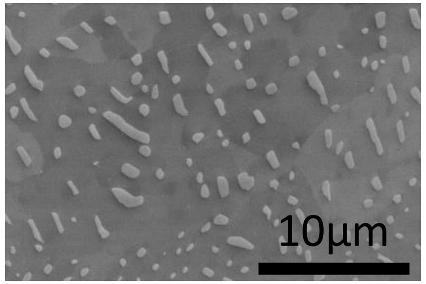
→ **ThermoCalc – Python rapid screening of vast design space**

Also:

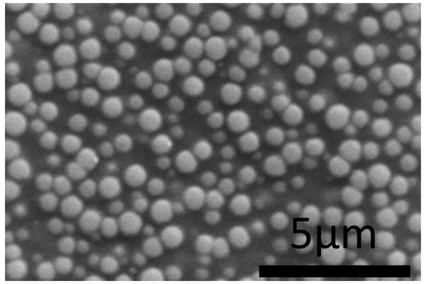
- Mechanical properties
- Solidification under laser melting

	Nb_{70}	Mo_{70}	$V_{35}Mo_{35}$	$Nb_{35}Mo_{35}$	$Nb_{35}Ta_{35}$	$Mo_{35}Ta_{35}$
$Ru_{15}Hf_{15}$	>1900°C	>1900°C	>1900°C	>1900°C	>1900°C	>1900°C
$Ru_{15}Ti_{15}$	1300-1600°C	1750-1900°C	1600-1750°C	1750-1900°C	1300-1600°C	single BCC
$Ru_{15}Al_{15}$	BCC + sigma	>1750°C	1300-1600°C	>1750°C; + A15 at 1300°C	BCC + sigma	>1750°C; + A15 at 1300°C

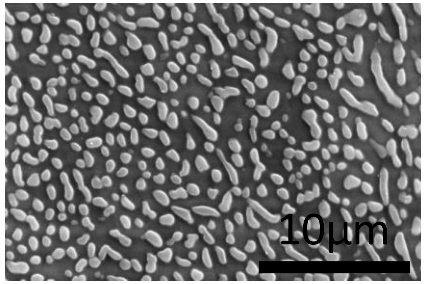
$Ru_{15}Ti_{15}$ - Nb_{70}



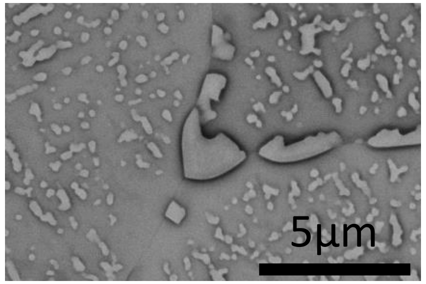
$Ru_{15}Ti_{15}$ - $V_{35}Mo_{35}$



$Ru_{15}Ti_{15}$ - $Nb_{35}Mo_{35}$



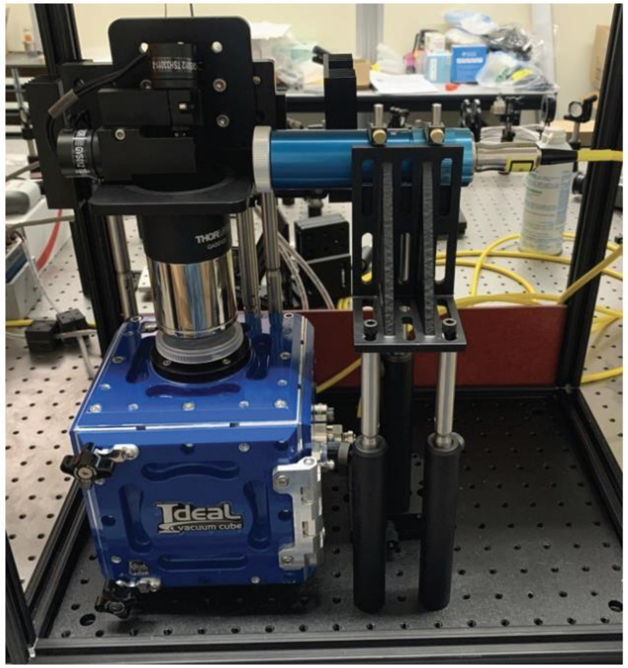
$Ru_{15}Al_{15}$ - $V_{35}Mo_{35}$

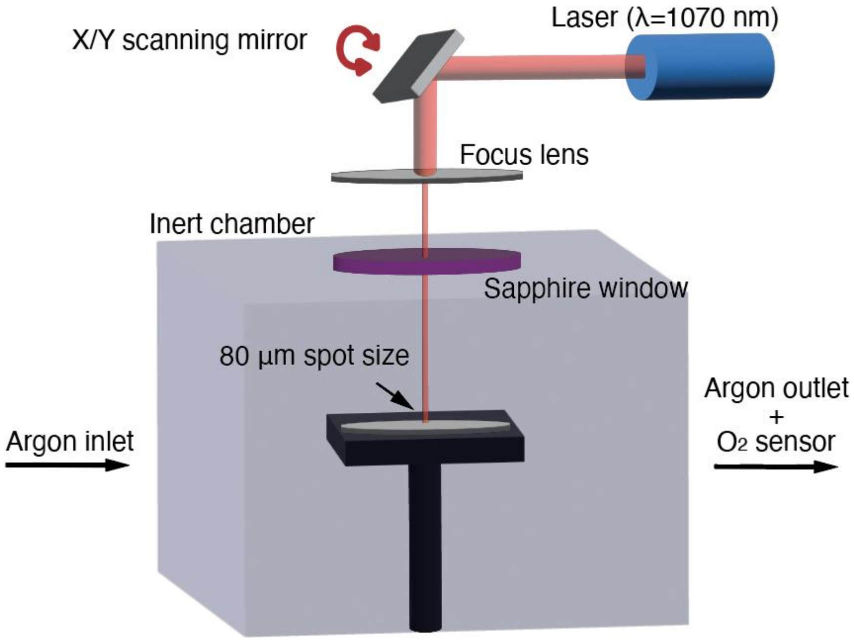


TC-Python used to predict solidification characteristics

Lead: Kaitlyn Mullin, UCSB

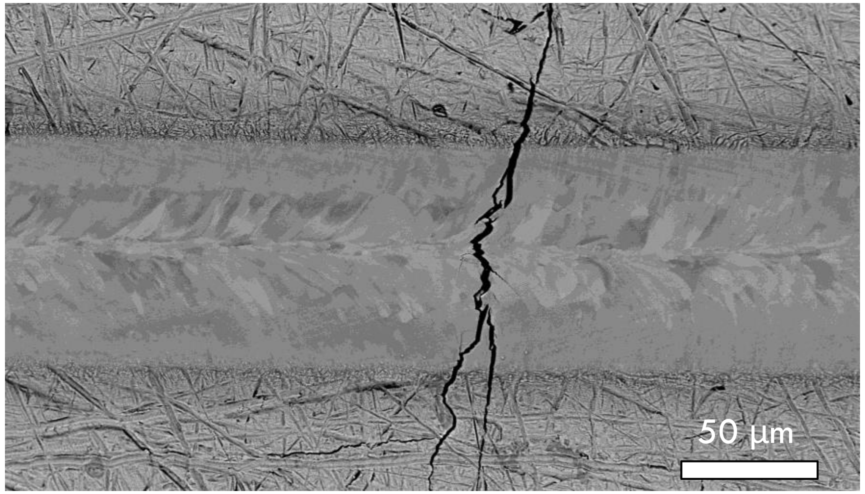
What is the influence of composition on crack susceptibility during printing?



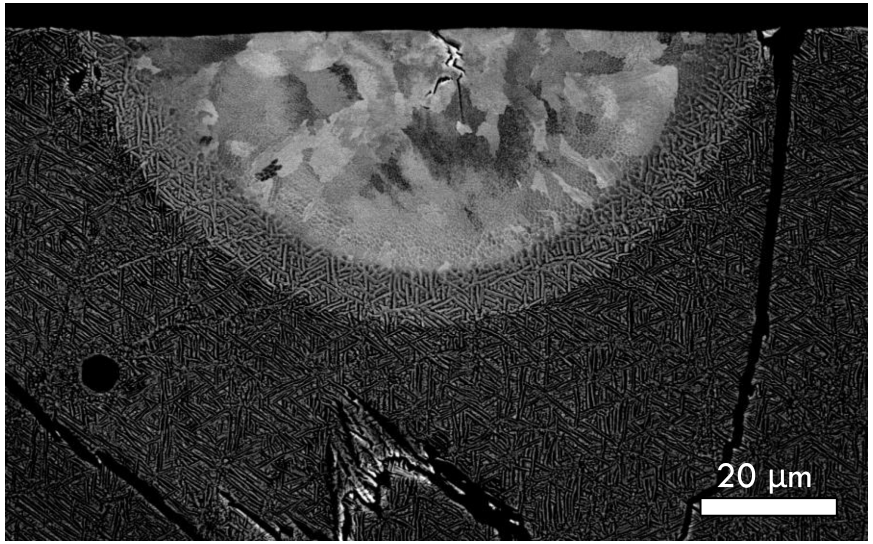


Example: 230 W, 200 mm/s laser melt of $Mo_{70}Al_{15}Ru_{15}$

Laser melted surface



Melt pool cross section

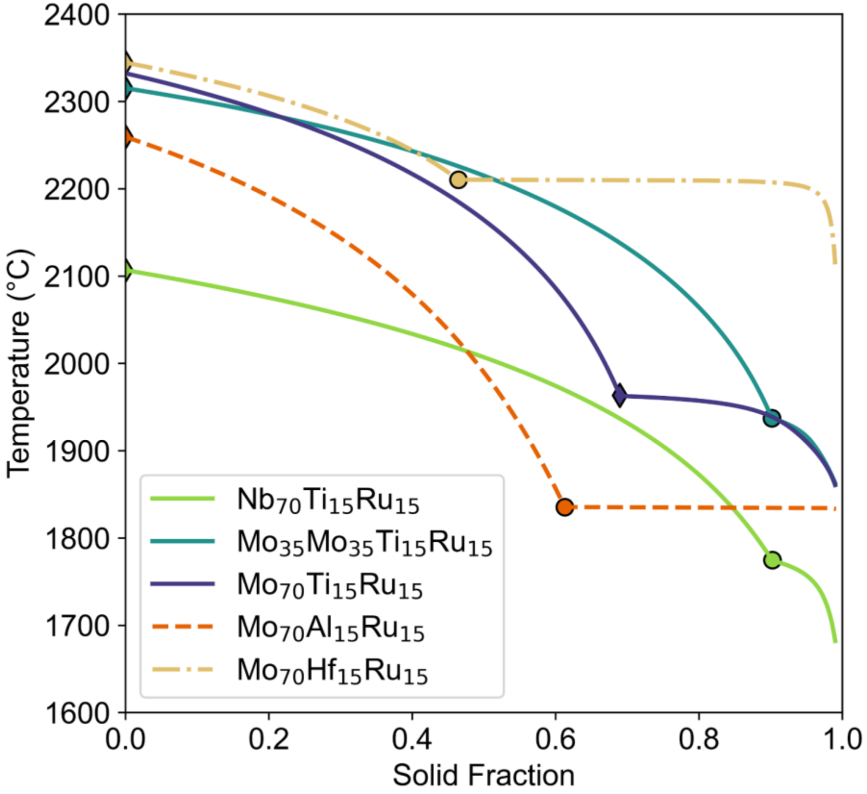


K. Mullin, T. Pollock et al. / Materials & Design 238 (2024):
[Rapid screening of single phase refractory alloys under laser melting conditions]

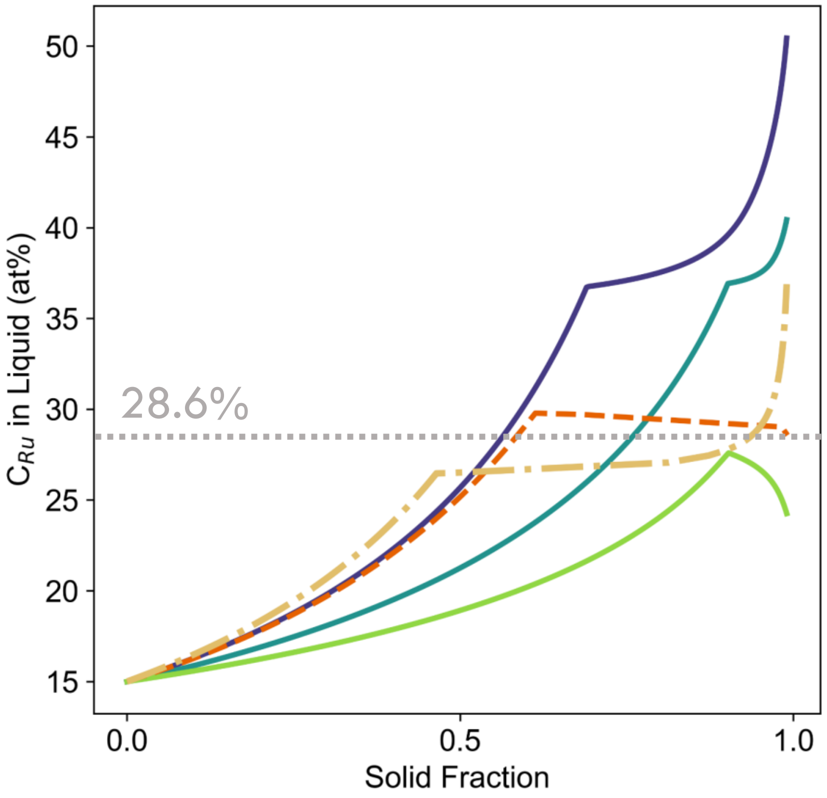
TC-Python used to predict solidification characteristics

"Scheil Calculations"

Solidification freezing range

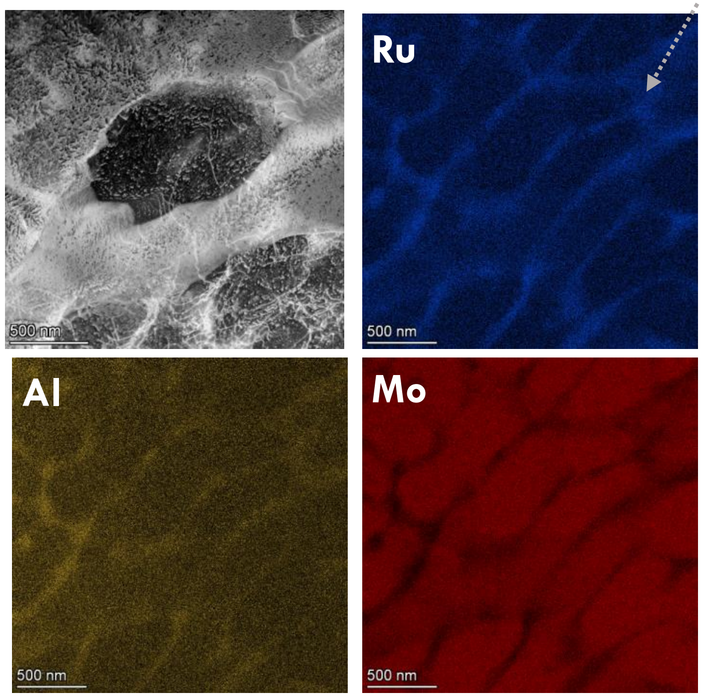


Partitioning behavior



STEM-EDS of laser melted $Mo_{70}Al_{15}Ru_{15}$

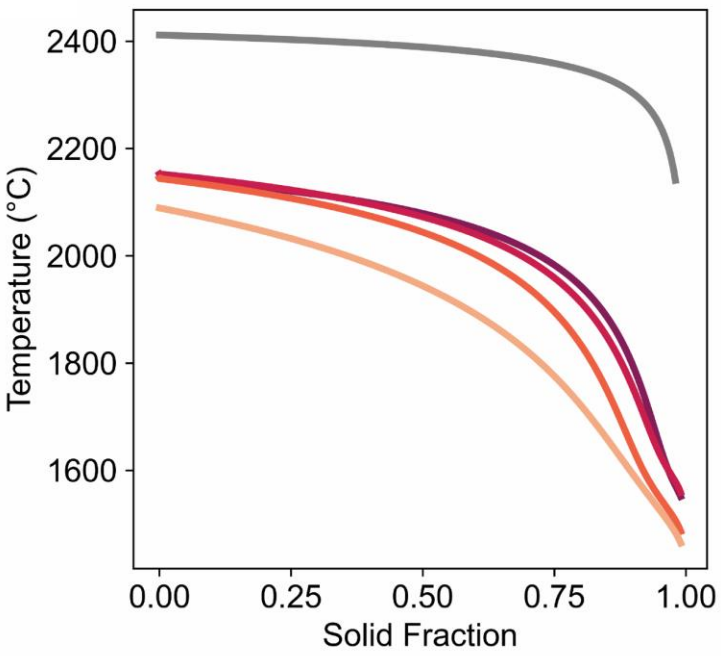
29.4at.%



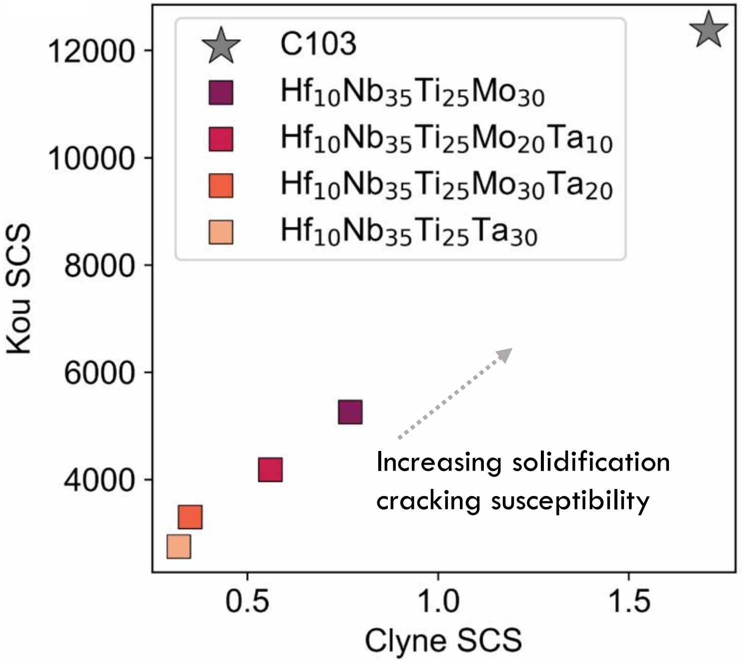
K. Mullin, S.A. Kube, S. Wu, T. Pollock (2024, under review):
Cracking and precipitation behavior of refractory BCC-B2 alloys under laser melting conditions

TC-Python used to predict solidification characteristics

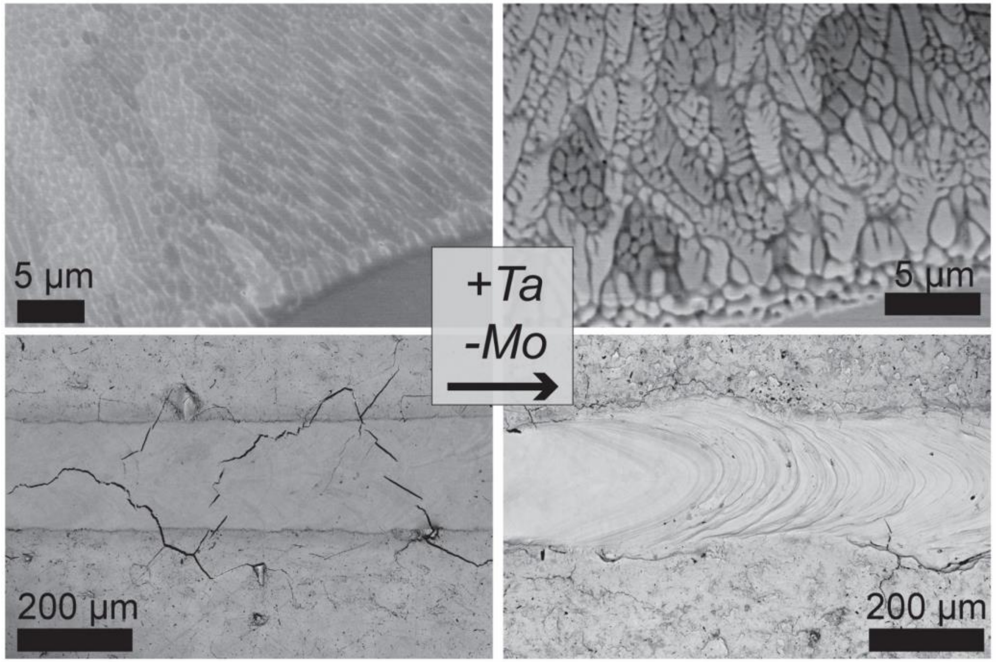
ThermoCalc Scheil curve compositional sweep



Predictive criteria from Scheil curves



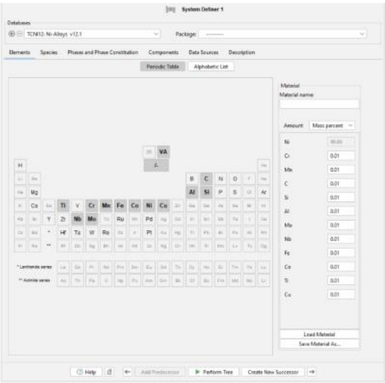
Rapid laser screening experiments

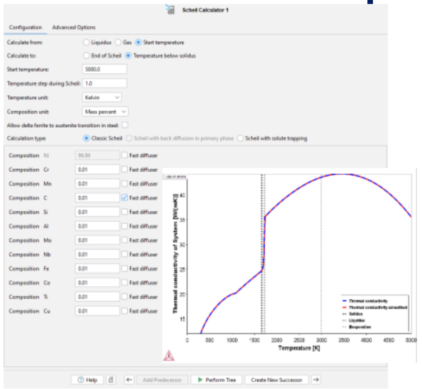


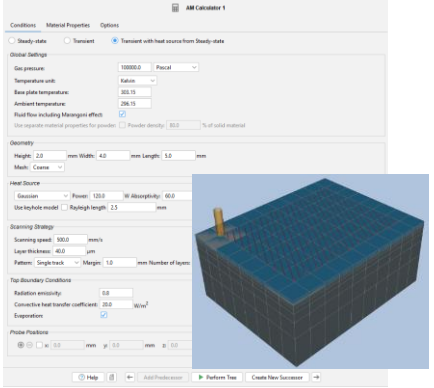
K. Mullin, T. Pollock et al. / Materials & Design 238 (2024):
[Rapid screening of single phase refractory alloys under laser melting conditions]

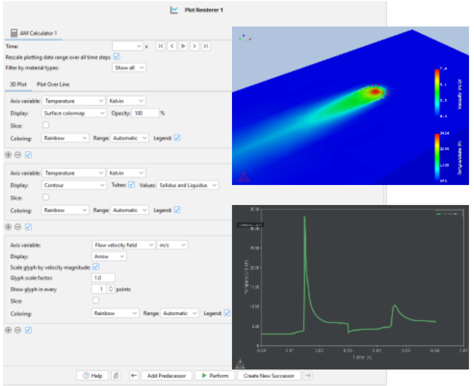
Additive Manufacturing (AM) Module
Unified Treatment of Material Properties and Process Parameters

Thermo-Calc Software









Precipitation

Diffusion

System Definer → Extended Scheil Calculation → AM Module → Post Processing → Export Results

System Definer

Define alloy system, retrieve Thermodynamic and Thermophysical data

Extended Scheil Calculation

Extraction of materials properties from evaporation down to RT including solidification segregation.

Obtain enthalpy, heat capacity, density, thermal conductivity, viscosity, surface tension,volume, molar mass of gas and driving force for evaporation

AM Module

Simulate AM with parameters such as: Laser power, Scanning speed and Strategy Layer thickness, Base plate temperature.

Takes into account: Thermal conduction and Fluid flow, Powder density, and heat losses due to radiation and convection and evaporation

Post Processing

Visualize in 3D, over a selected line or at a chosen point over time.

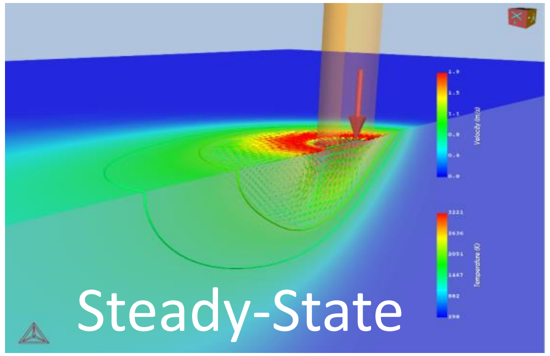
Plottable quantities: Temperature, Flow velocity, Surface tension,Thermal conductivity, Dynamic viscosity and Melt Pool dimension.

Export Results

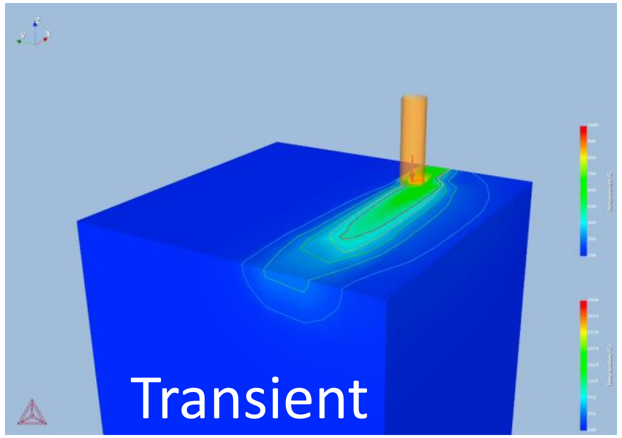
Export time-temperature profile, melt pool dimension and/or temperature distribution in space to other Thermo-Calc add-on Modules like DICTRA or TC-PRISMA, or to other external computational softwares.

Additive Manufacturing (AM) Module
Unified Treatment of Material Properties and Process Parameters

- ✔ Fe-alloys
- ✔ Ni-base Superalloys
- ✔ HEAs
- ✔ Ti-alloys
- ✔ Al-alloys
- ✔ Mg-alloys
- ✔ Cu-alloys
- ✔ Noble-alloys



- ✔ Size of melt pool
- ✔ Fluid flow
- ✔ Peak temperature
- ✔ Property variation through melt pool
- ✔ More...



- ✔ All above vs time
- ✔ T vs time in build
- ✔ Connect with Diffusion and/or Precipitation Module

Q&A

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Full length article

Navigating the BCC-B2 refractory alloy space: Stability and thermal processing with Ru-B2 precipitates

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A R T I C L E I N F O

Keywords:
High temperature materials
Precipitation strengthening
Refractory multi principal element alloys
Thermal processing
B2 phase
Calphad
Combinatorial

A B S T R A C T

Refractory multi-principal element alloys (RMPEAs) could provide next-generation high temperature alloys, but their ductility and high temperature strength need significant improvement. Emulating superalloy γ-γ' micro-structures, RMPEAs combining a ductile BCC matrix with embedded B2 precipitates for strengthening could meet this goal. Two-phase BCC-B2 RMPEAs have recently been demonstrated, but the B2 phase typically exhibits insufficient thermodynamic stability for operating temperatures ≥1300 °C.

Using high-throughput CALPHAD predictions, we screen across 3,500 potential BCC-B2 systems. Promising compositions are predicted for alloys combining Ru-based B2s with refractory BCC elements. A total of 20 such

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