



Thermo-Calc Software
Release News
Version 2024b

Release Highlights

- ▶ **Additive Manufacturing Module**
 - ✓ Improves Keyhole Model with Fluid Flow
 - ✓ Adds Batch and Grid Calculation Types
 - ✓ Adds Printability Maps

- ▶ **New Titanium Model Library**

- ▶ **Elastic Properties Introduced**

- ▶ **Significant Speed Improvements in Property Calculations**

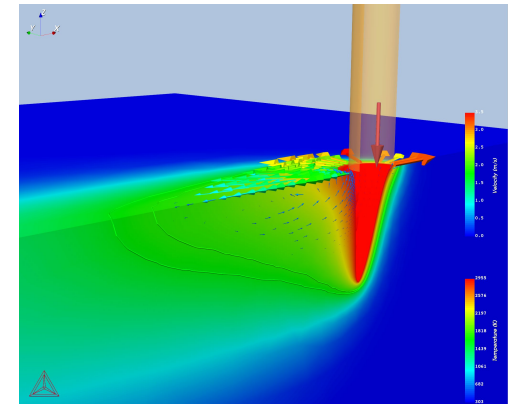
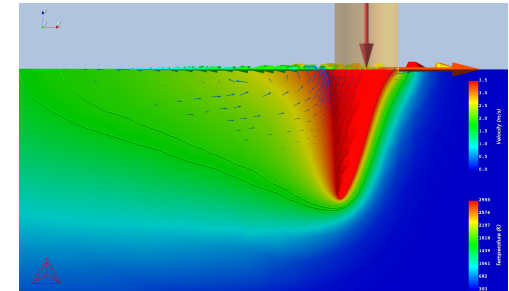
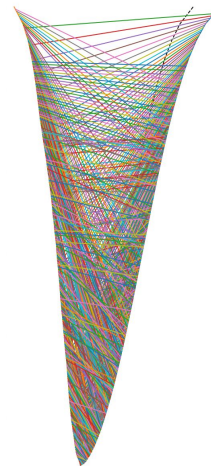
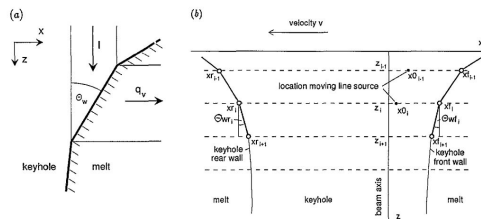
- ▶ **Improved Martensitic Steel Strength Property Model**

- ▶ **First ever databases for Molybdenum-based and Niobium-based refractory alloys**

- ▶ **Five other new databases**

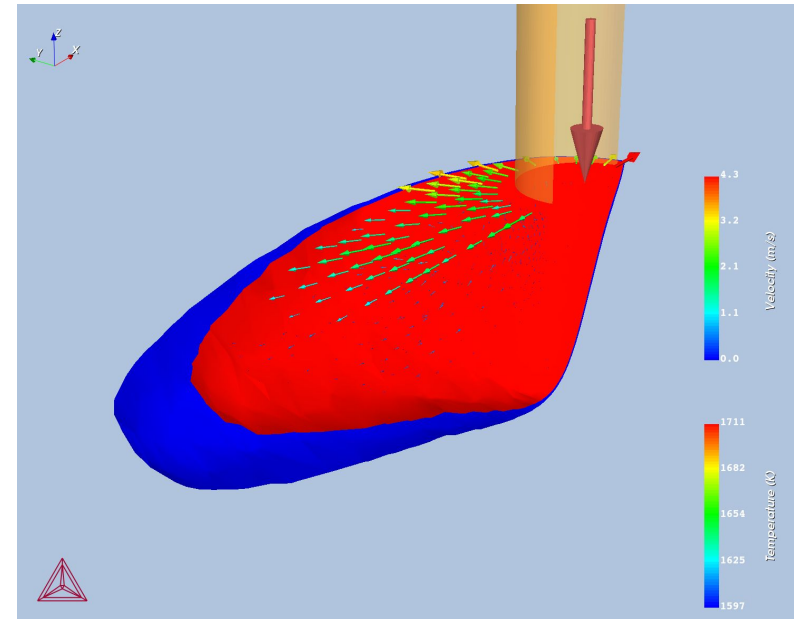
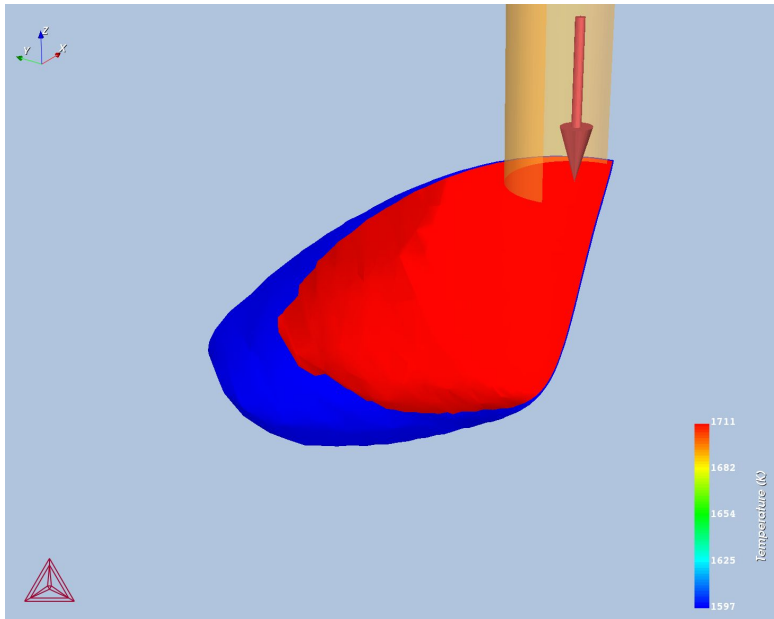
Keyhole Model

- Gaussian heat source at surface
- Geometry of keyhole calculated as a pre-step and cut out from mesh
- Steady-state simulation performed on mesh
- Secondary reflections implemented
- Now with fluid flow!



Fluid Flow Can Make the Melt Pool Wider and Longer

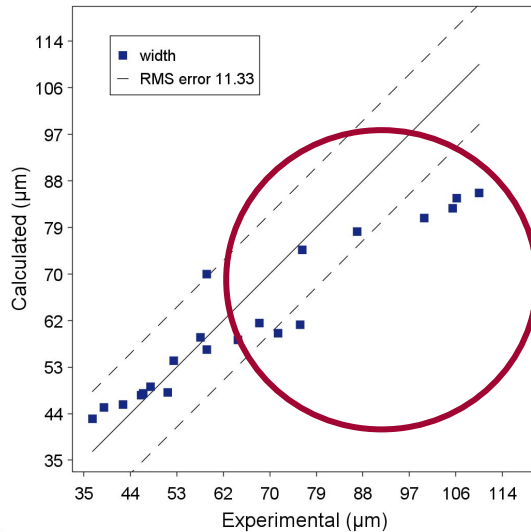
316L: P50W v=400mm/s



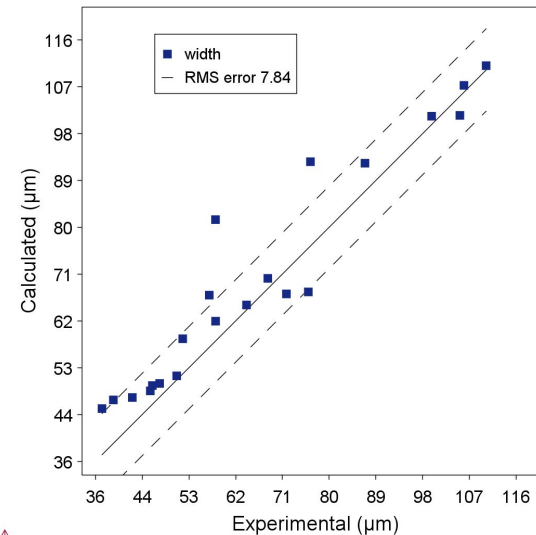
Effect of Fluid Flow - SS316L Hu et al. 2019*

- Gaussian beam radius 22 μm
- Absorptivity 30%

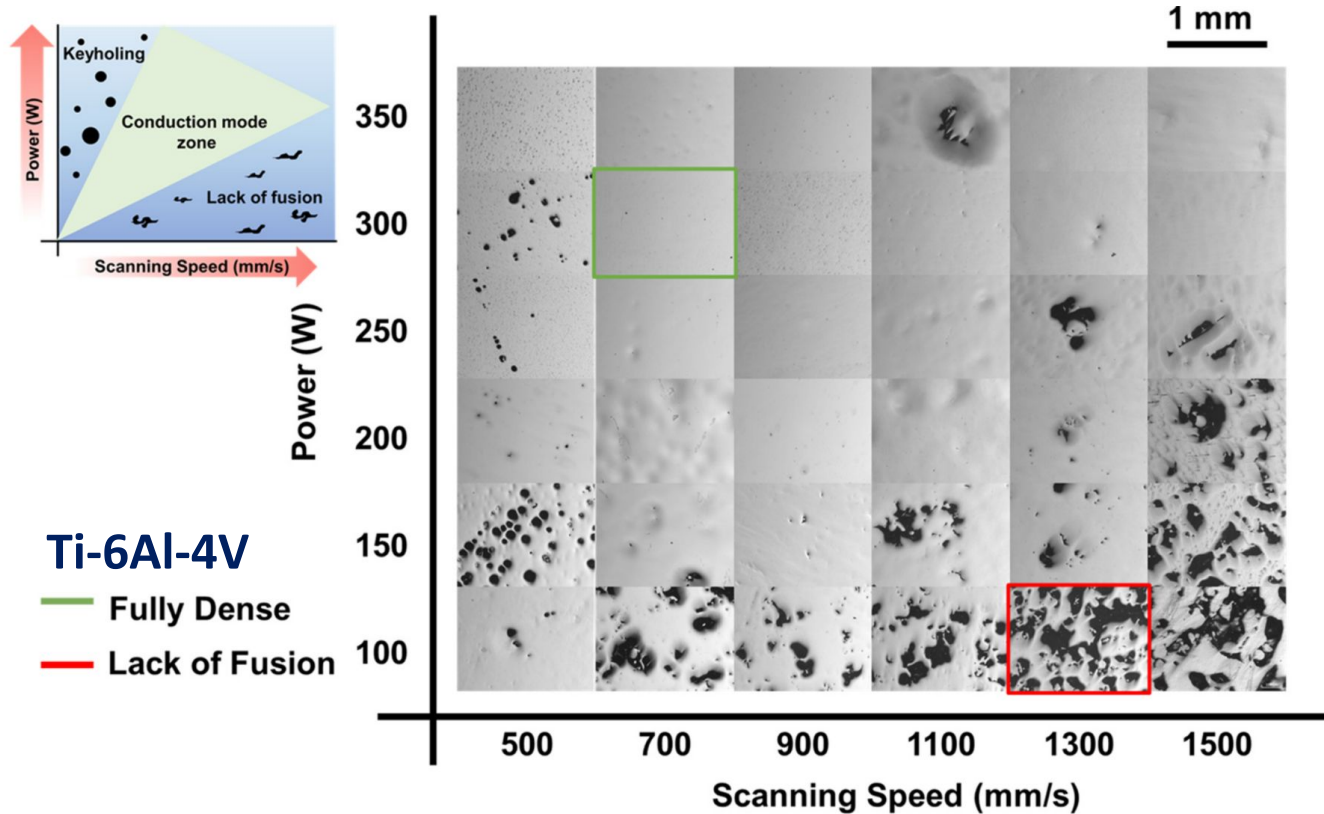
Without fluid flow



With fluid flow



Printability Maps (aka Process Maps)



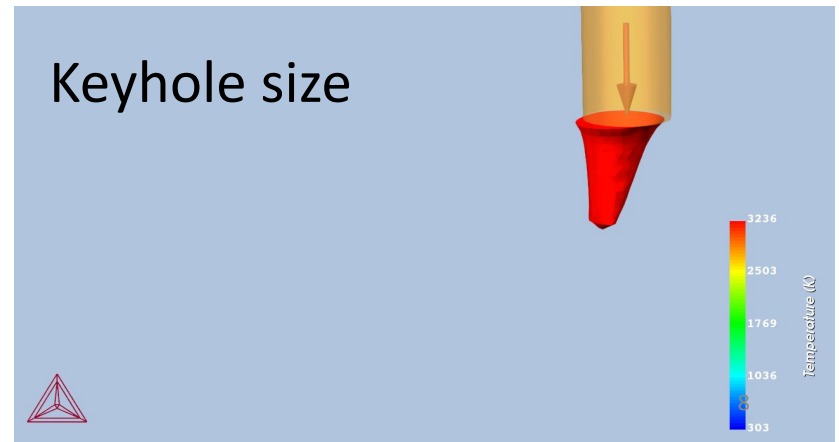
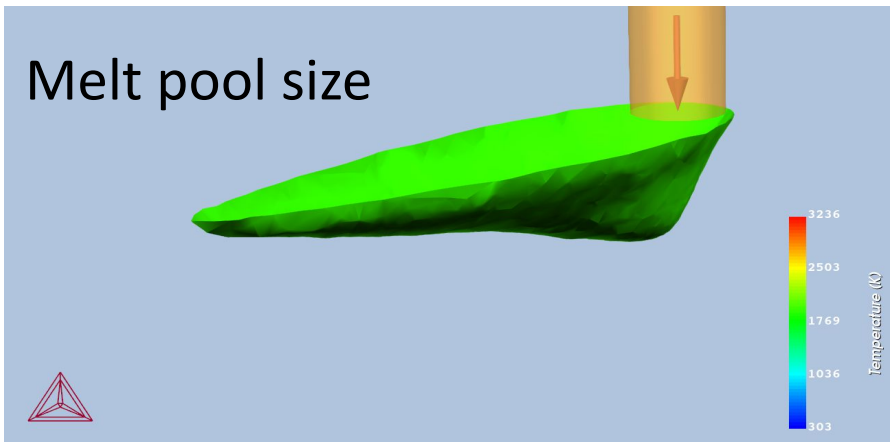
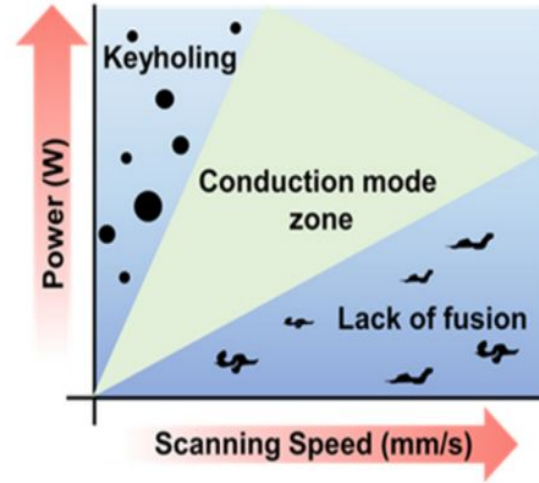
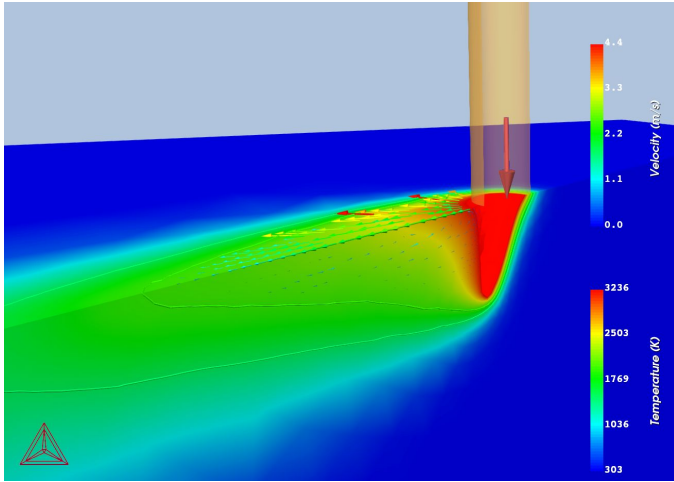
Convergence of Steady-state Models Improved

- A new adaptive mesh criterion refines the mesh based on the temperature gradient.
- Improvements in the Streamline upwind Petrov - Galerkin (SUPG) stabilization scheme.

Fluid Flow Model Improved for Turbulent Conditions

- A new subgrid model that relies on the eddy-viscosity assumption is applied to account for unresolved turbulent motions that cannot be directly simulated due to computational limitations.
- The Smagorinsky model is now applied as default, and it provides a simple way to estimate *Subgrid-scale (SGS)* viscosity in a large eddy simulation

2024b Additive Manufacturing (AM) Module Printability Maps

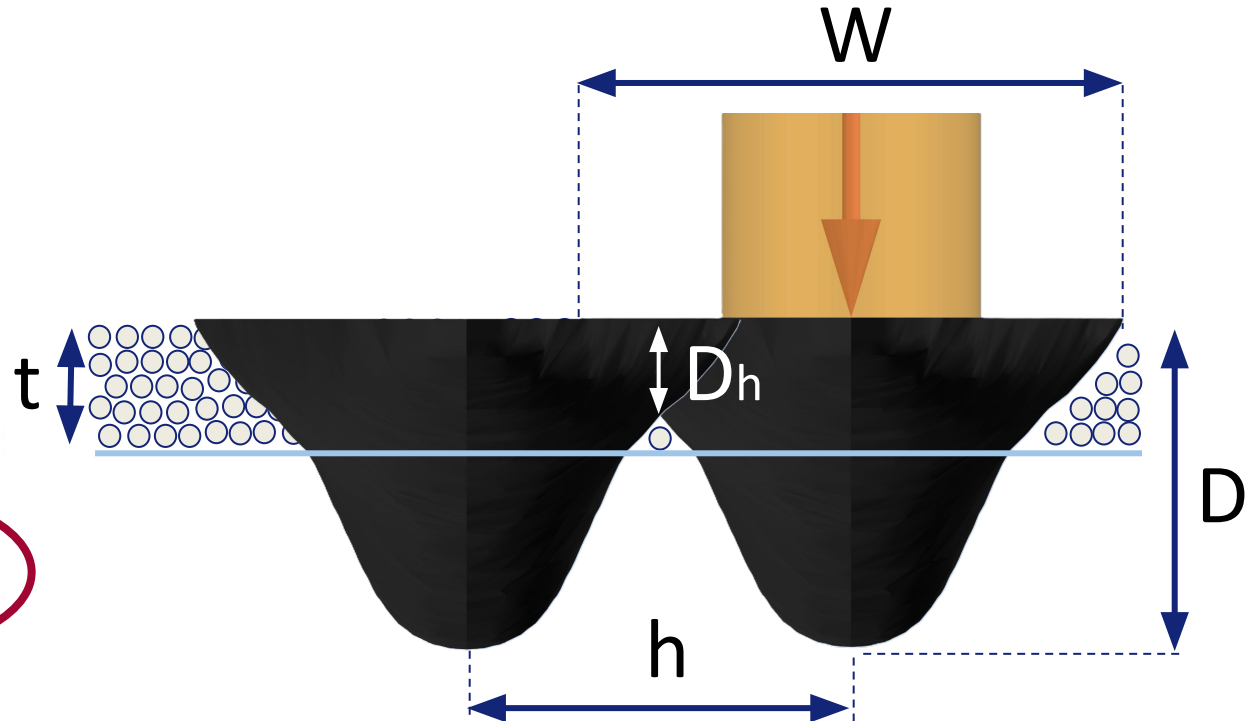
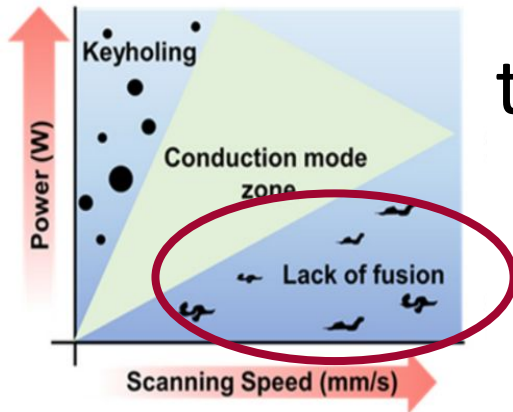


Printability Maps: Lack of Fusion Porosity

Lack of fusion criteria:

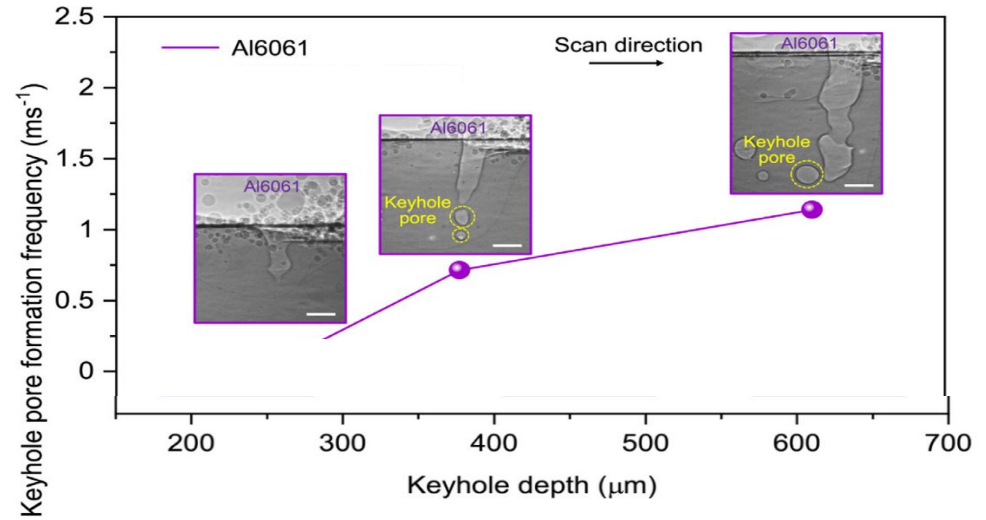
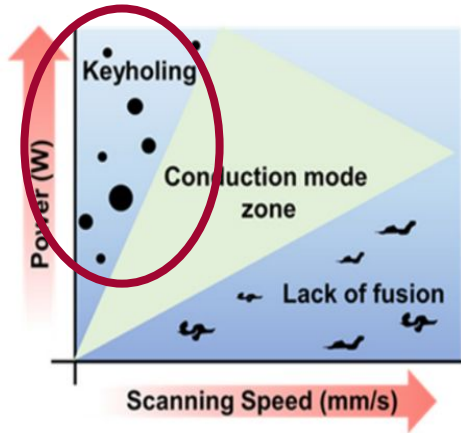
- D/t
- Dh/t

Uneven porosity



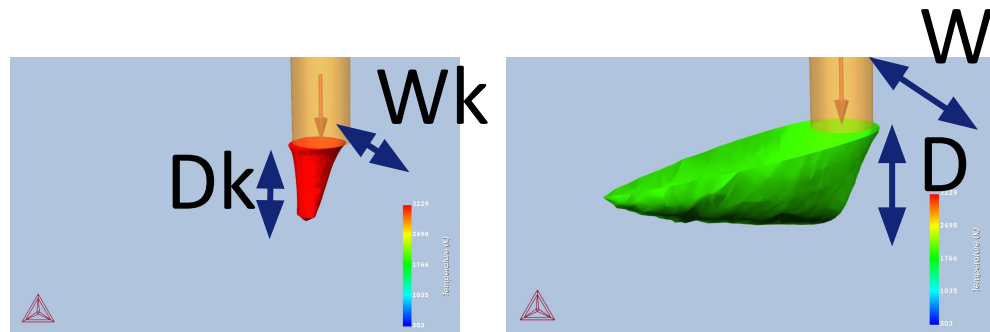
Printability Maps: Keyhole Porosity

Round porosity



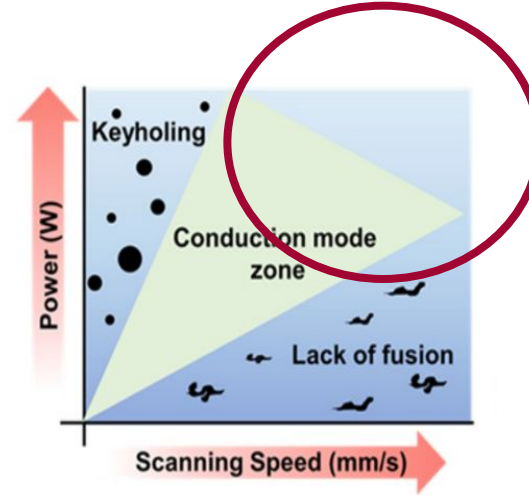
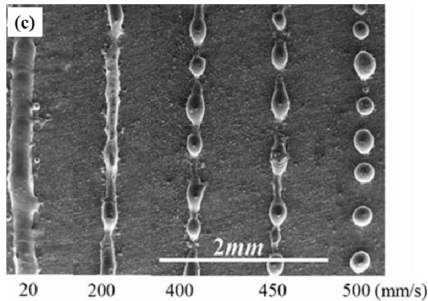
Keyhole criteria:

- Wk/Dk
- W/D



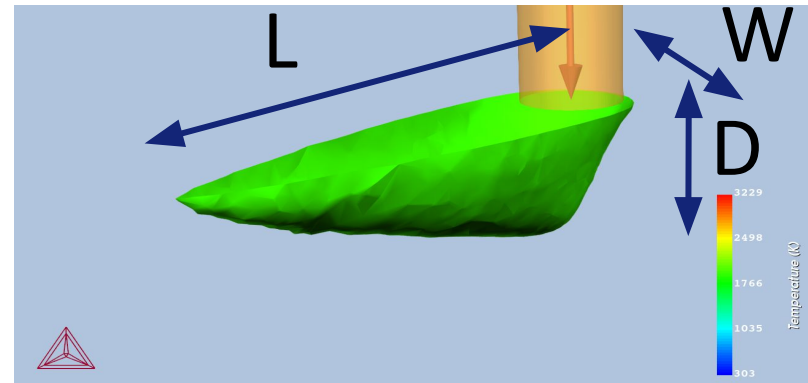
Printability Maps: Balling

Balling defects



Balling criteria:

- W/L
- D/L



Batch and Grid Calculations: Run Many Steady-state Calculations

- Batch

Calculation Type

Single Point
 Heat Source Calibration
 Batch
 Grid

Batch Experiment Data

Experiment file delimiter Comma

#	Power (W)	Speed (mm/s)	P/V (J/mm)	Exp.width (µm)	Exp.depth (µm)	Use
1	60.000000	2400.000000	0.025000	36.842110	9.444444	<input checked="" type="checkbox"/>
2	60.000000	2000.000000	0.030000	39.009290	10.555560	<input checked="" type="checkbox"/>
3	50.000000	1200.000000	0.041667	51.075950	9.303797	<input checked="" type="checkbox"/>
4	60.000000	1600.000000	0.037500	46.439630	11.666670	<input checked="" type="checkbox"/>
5	80.000000	2800.000000	0.028571	42.621560	9.279661	<input checked="" type="checkbox"/>
6	90.000000	2800.000000	0.032143	46.046510	11.949150	<input checked="" type="checkbox"/>
7	60.000000	1200.000000	0.050000	52.215190	12.109700	<input checked="" type="checkbox"/>
8	50.000000	800.000000	0.062500	57.272730	27.931030	<input checked="" type="checkbox"/>
9	100.000000	2800.000000	0.035714	47.822410	14.364410	<input checked="" type="checkbox"/>
10	40.000000	400.000000	0.100000	58.461540	14.545450	<input checked="" type="checkbox"/>

- Grid

Calculation Type

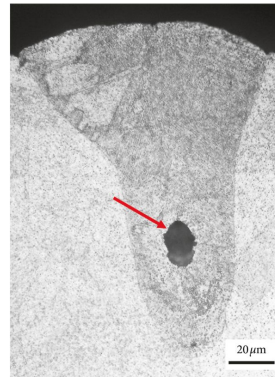
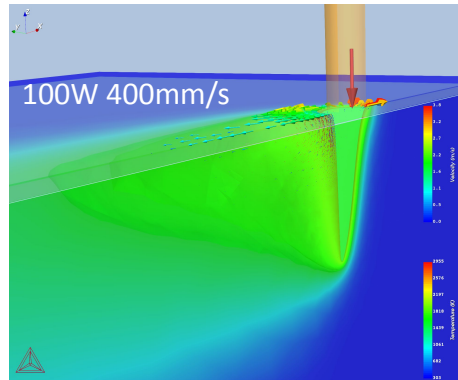
Single Point
 Heat Source Calibration
 Batch
 Grid

Grid Definitions

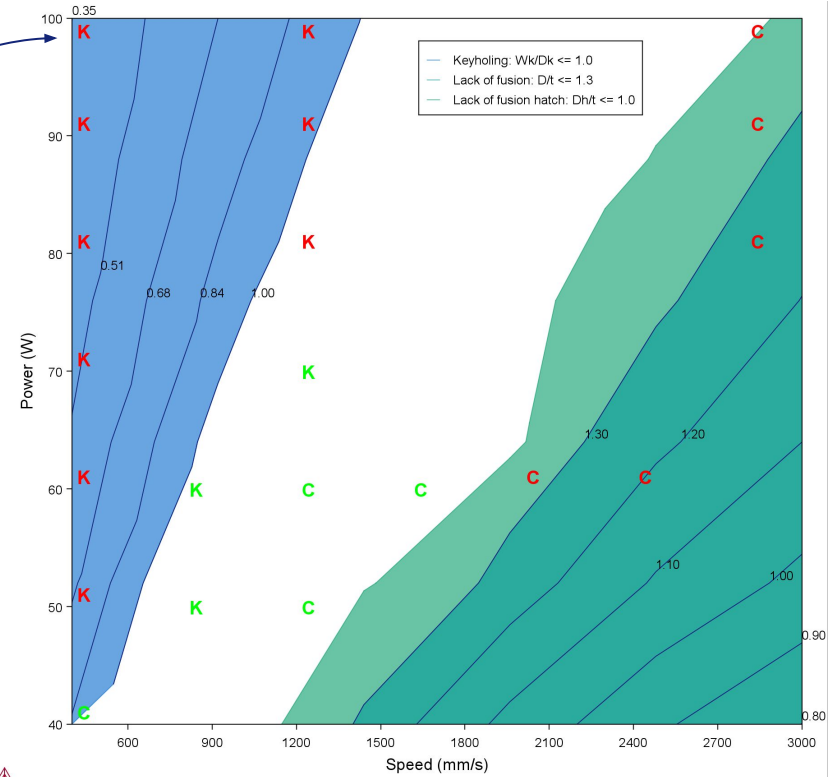
Quantity	Min	Max	Number of steps
Power (W)	<input type="text" value="50.0"/>	<input type="text" value="200.0"/>	<input type="text" value="5"/> <input type="button" value="↕"/>
Scanning speed (mm/s)	<input type="text" value="500.0"/>	<input type="text" value="1200.0"/>	<input type="text" value="5"/> <input type="button" value="↕"/>

SS316L Hu et al. 2019*

- Gaussian beam radius 22 μm
- Powder layer thickness 10 μm
- Absorptivity 30%

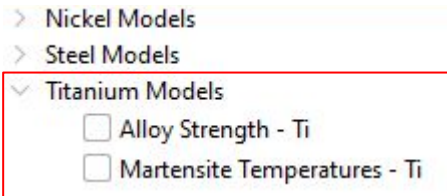


Ex. AM_09a_Printability_Map_316L



New Titanium Property Model Library

- Together with the update to TCTI6 we focus on a new Property Model Library for Titanium alloys.



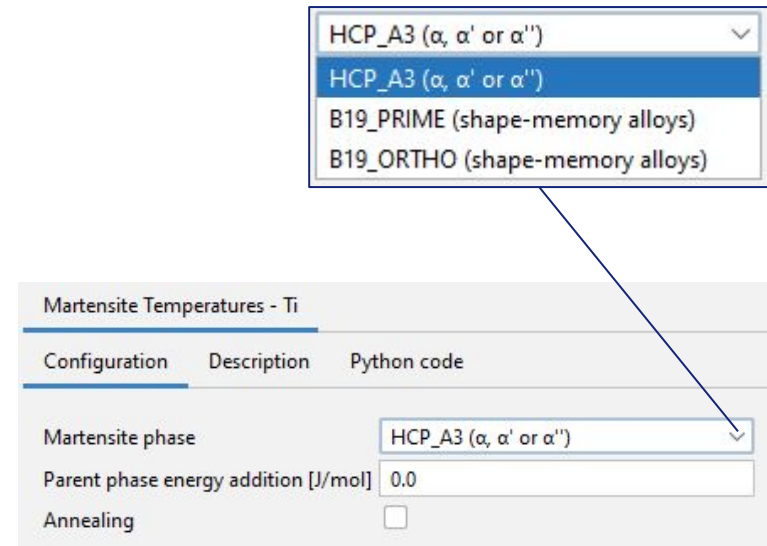
PM_Ti_01_Martensite_Temperature_s_Ti-Zr.tcu



PM_Ti_02_Alloy_Strength_Ti-O.tcu

Titanium Model Library: Martensite Temperatures - Ti

- New Property Model for calculating the Ms temperature for Titanium alloys.
 - Developed for structural and shape-memory alloys.
 - Considers three different martensitic phases.
 - Based on the T-Zero Temperature and a composition-dependent correction.
 - Parent phase stability can be displaced by a value or function input.
 - The annealing checkbox allows for evaluating the composition of the parent phase, in case of multi-phase alloy compositions.

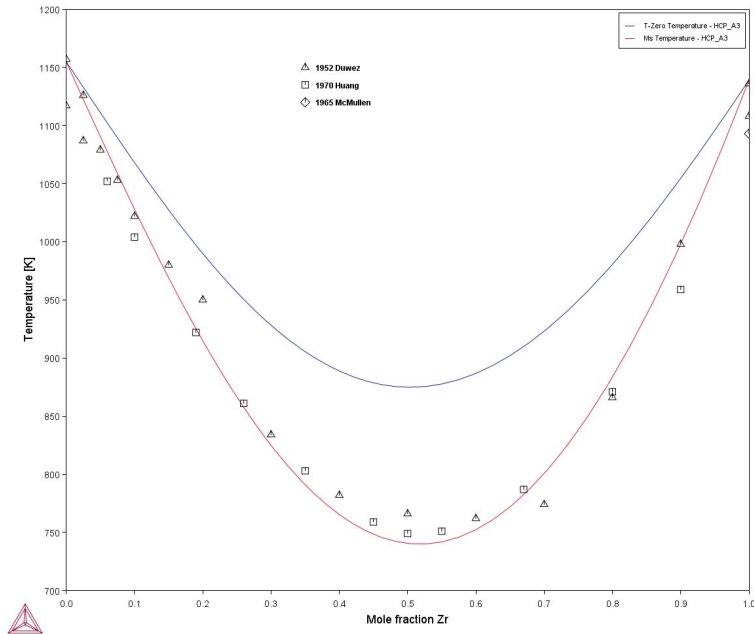


Martensite Temperatures - Ti

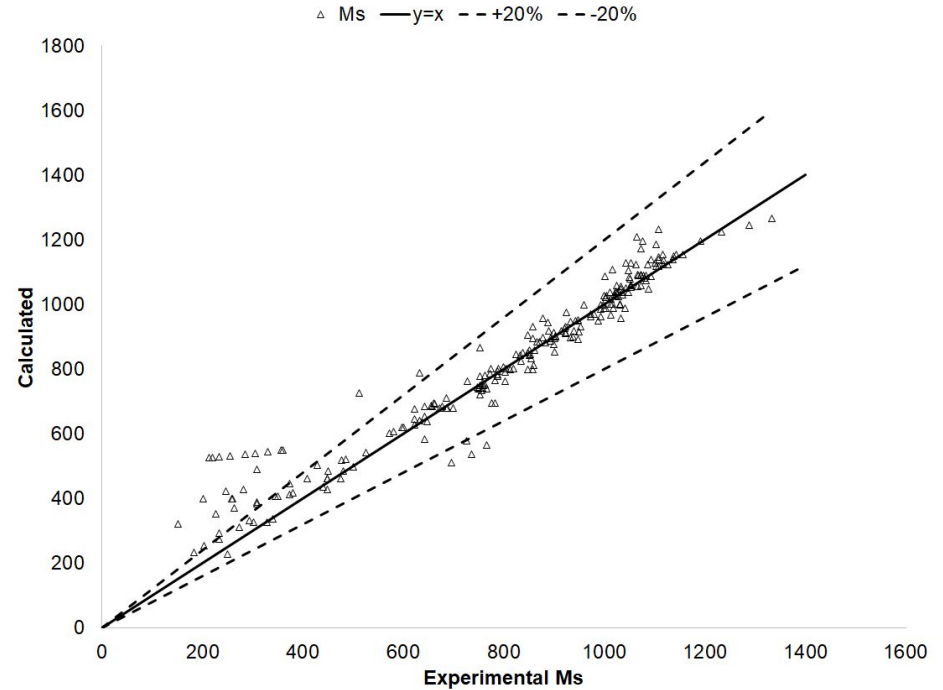
Configuration	Description	Python code
Martensite phase	HCP_A3 (α, α' or α'')	
Parent phase energy addition [J/mol]	0.0	
Annealing	<input type="checkbox"/>	

Titanium Model Library: Martensite Temperatures - Ti

- Example: PM_Ti_01

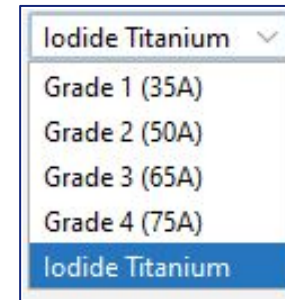


- Benchmark for alpha martensite.



Titanium Model Library: Alloy Strength - Ti

- New strength Property Model.
 - Developed using a large dataset.
 - Impurity contents are of high importance!
Select appropriate base grade!
 - All binary Ti-X contributions to solid solution strengthening are parameterized.
 - Also considers grain boundary and precipitation strengthening.
 - Effect of temperature on dislocation mobility (softening) is considered.



Alloy Strength - Ti

Configuration	Description	Python code
Titanium base grade		Iodide Titanium
Evaluation Temperature		300.0
Grain boundary strengthening		<input checked="" type="checkbox"/>
Grain size [um]		100.0
User-defined Hall-Petch coefficient		<input type="checkbox"/>
Precipitation strengthening		<input type="checkbox"/>
Constant strength addition		0.0

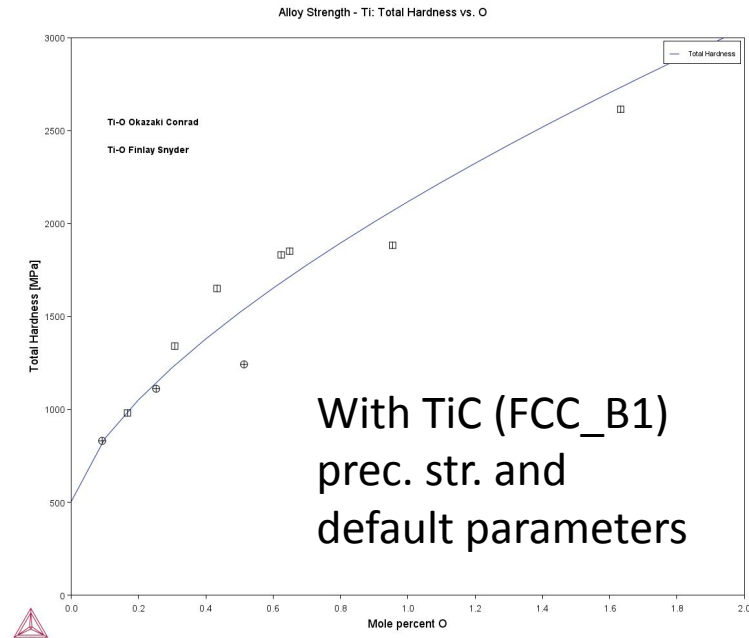
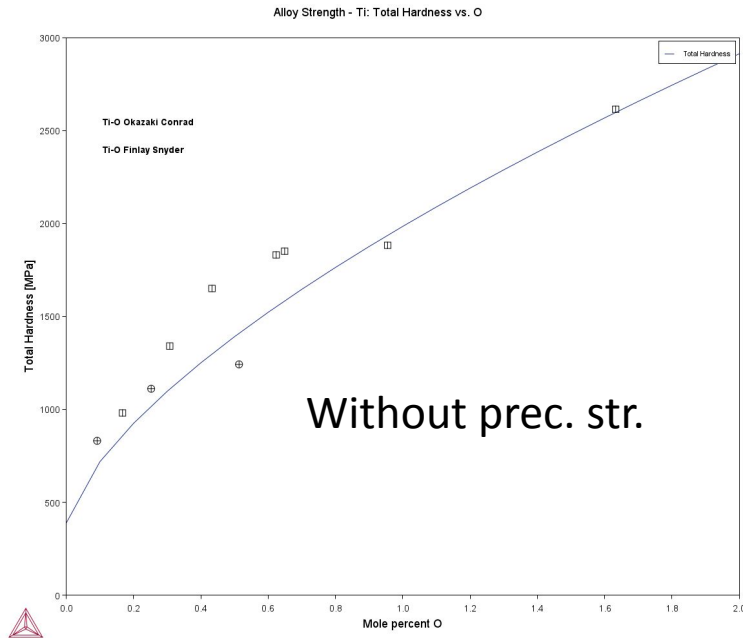
Titanium Model Library: Alloy Strength - Ti

- Making use of modeled elastic properties in the thermodynamic database TCTI6:

Alloy Strength - Ti		
Configuration	Description	Python code
Titanium base grade	Iodide Titanium	▼
Evaluation Temperature	298.15	
Grain boundary strengthening	<input type="checkbox"/>	
Precipitation strengthening	<input checked="" type="checkbox"/>	
Precipitate phase	FCC_B1	▼
Precipitate radius	1.0E-8	
Critical radius	1.0E-8	
Taylor factor	3.0	
Shear modulus	Calculated	
Burgers vector	2.5E-10	
Constant strength addition	0.0	

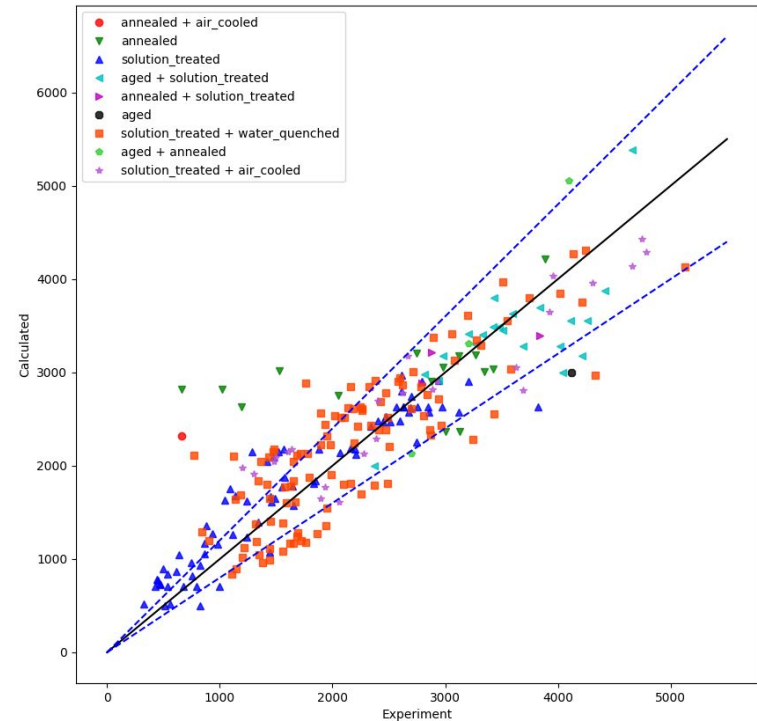
Titanium Model Library: Alloy Strength - Ti

- Example: PM_Ti_O2



Titanium Model Library: Alloy Strength - Ti

- Benchmark versus a multitude of alloys (Hardness in MPa).
- Some scatter due to:
 - Complex heat treatments.
 - Unknown or ill-determined impurity levels.
 - Non negligible dislocation density due to martensite or deformed grains.
- Trends with respect to all elements have been thoroughly checked and look good!



Parallelization of Property Models

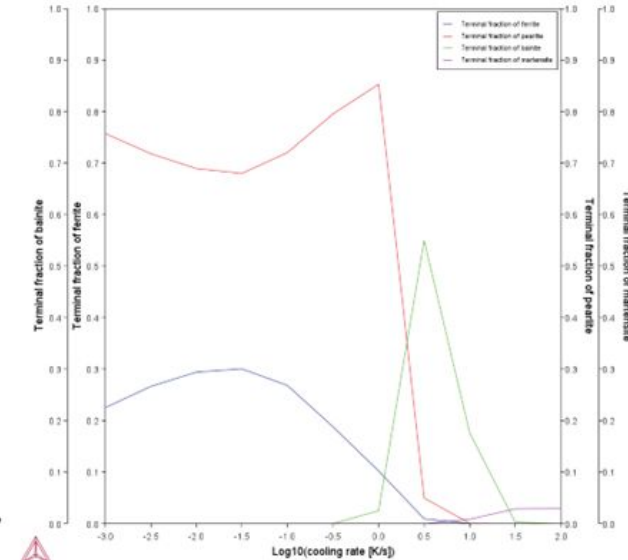
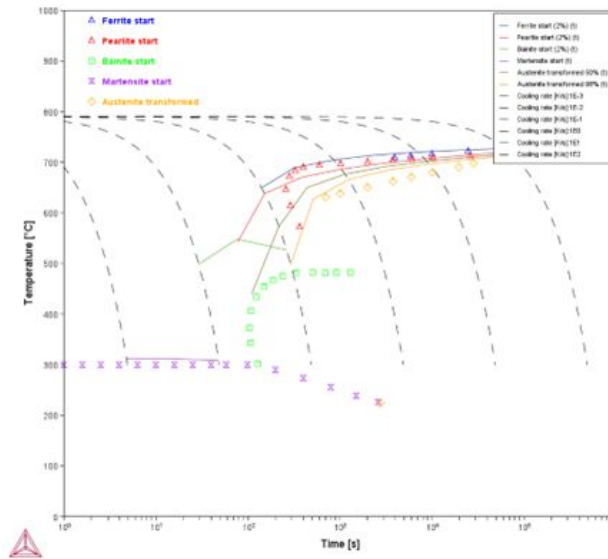
Windows 10 Pro

i9-7920X @ 2.9Ghz, 12 cores

64 GB RAM

PM_Fe_08 CCT

- 33 mins total calculation time with parallelization, 10 workers
- > 10 hours without



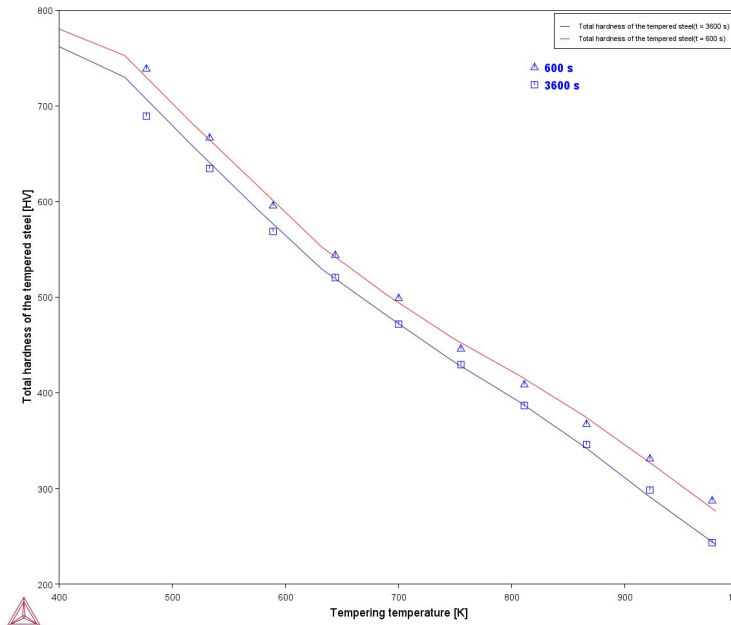
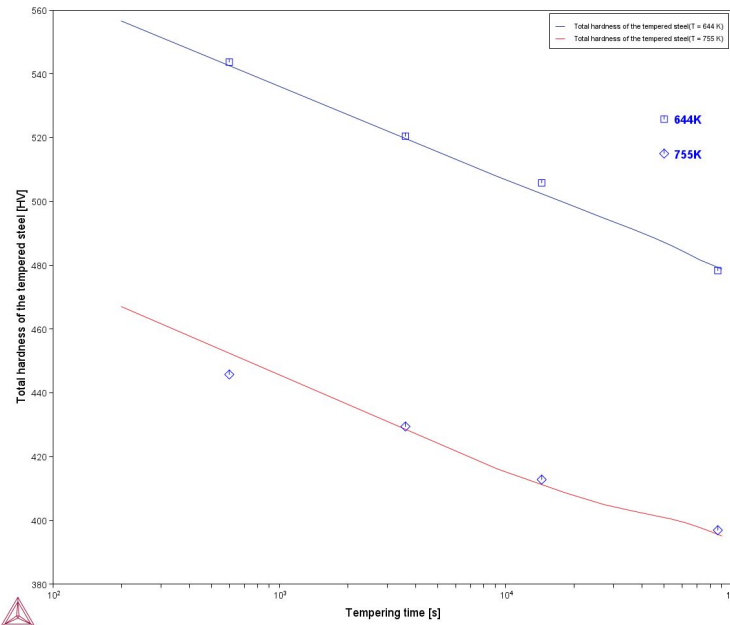
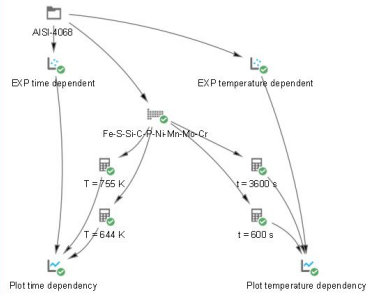
Steel Model Library: Improved Martensitic Steel Strength Model

- A large number of datapoints has been collected and curated.
- The tempering behavior has been deduced in detail using machine learning.
- Tempering time is now a parameter.
 - If a tempering time of 0 is given, the model will ignore the machine learning correction.
- Example is updated.

Martensitic Steel Strength		
Configuration	Description	Python code
Evaluation temperature		<input type="checkbox"/>
Annealing temperature		<input type="text" value="1273.15"/>
Quench temperature		<input type="text" value="298.15"/>
Tempering temperature		<input type="text" value="755.0"/>
Tempering time [s]		<input type="text" value="3600.0"/>
Suspend FCC, BCC or cementite		<input type="checkbox"/>
More options		<input type="checkbox"/>

Steel Model Library: Improved Martensitic Steel Strength Model

- Example: PM_Fe_10



Highlights

New Thermodynamic and Kinetic Databases

- 2 New! TCS Mo-based Alloys Databases (TCMO1 and MOBMO1)
- 2 New! TCS Nb-based Alloys Databases (TCNB1 and MOBNB1)

New Versions of Thermodynamic and Kinetic Databases

- TCS Ultra-high Temperature Materials Database (TCUHTM2)
- TCS Ti/TiAl-based Alloys Database (TCTI6)
- TCS Ti-alloys Mobility Database (MOBTI5)
- TCS Solder Alloy Solutions Database (TCSLD5)
- TCS Solder Alloy Solutions Mobility Database (MOBSLD2)

Other Updates:

- TCS Aluminum-based Alloys Database (TCAL9 to version 9.1)
- DEMO Solders Database SLDEMO

TCS Mo-based Alloys Database (TCMO1)

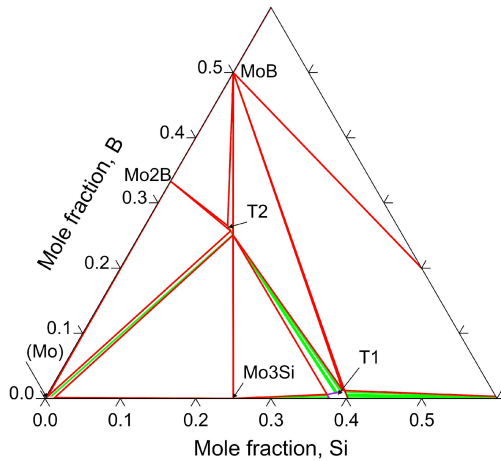
- ❑ 12 elements

Al	B	C	Cr	Fe	Hf	Mn	Mo	Re	Si	Ti	Zr
----	---	---	----	----	----	----	----	----	----	----	----

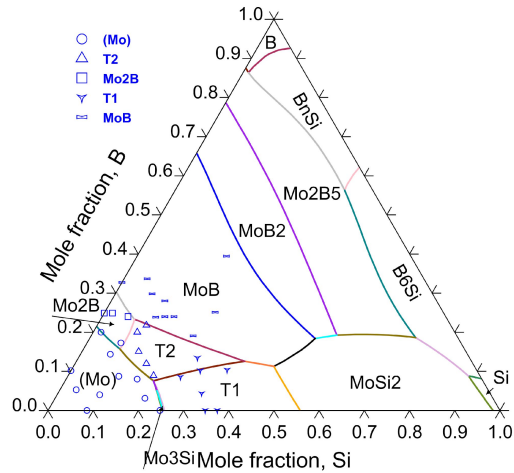
- ❑ 66 binary systems
- ❑ 46 ternary systems
 - 10 B-Mo-X ternary systems
 - 9 C-Mo-X ternary systems
 - 7 Mo-Si-X ternary systems
 - 20 other critical ternary systems
- ❑ 3 quaternary systems
 - B-Hf-Mo-Si, B-Mo-Si-Ti, B-Mo-Si-Zr
- ❑ 167 phases

TCS Mo-based Alloys Database (TCMO1)

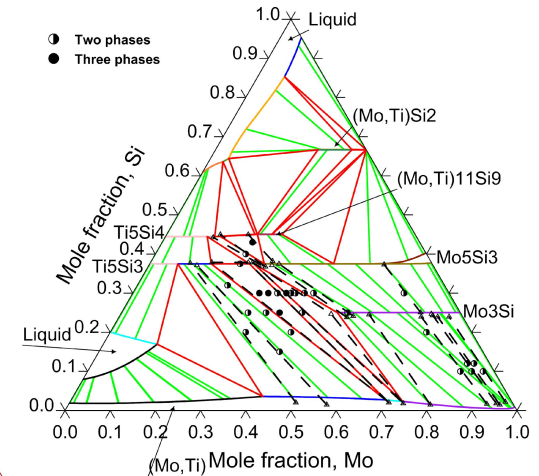
Ternary Phase Diagrams



B-Mo-Si: Isothermal section at 1600 °C



B-Mo-Si: Liquidus projection¹



Mo-Si-Ti: Isothermal section at 1600 °C²

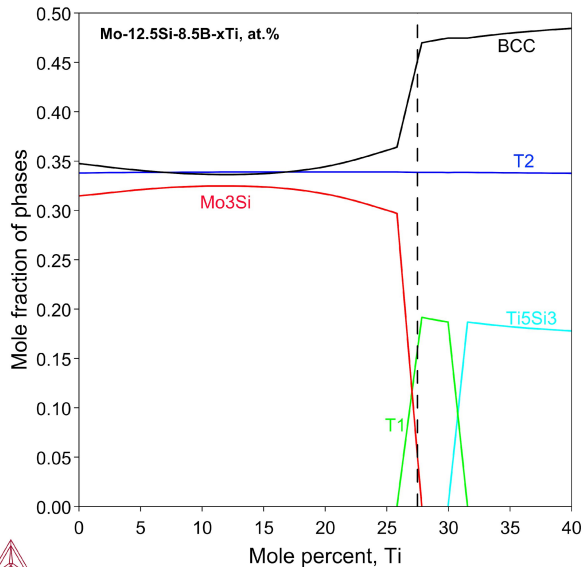
[1] Y. Yang, Y.A. Chang. Thermodynamic modeling of the Mo–Si–B system. *Intermetallics* 13 (2005) 121-128.

[2] Y. Yang, et al. Experimental investigation and thermodynamic descriptions of the Mo–Si–Ti system. *Materials Science and Engineering: A* 361 (2003) 281-293.

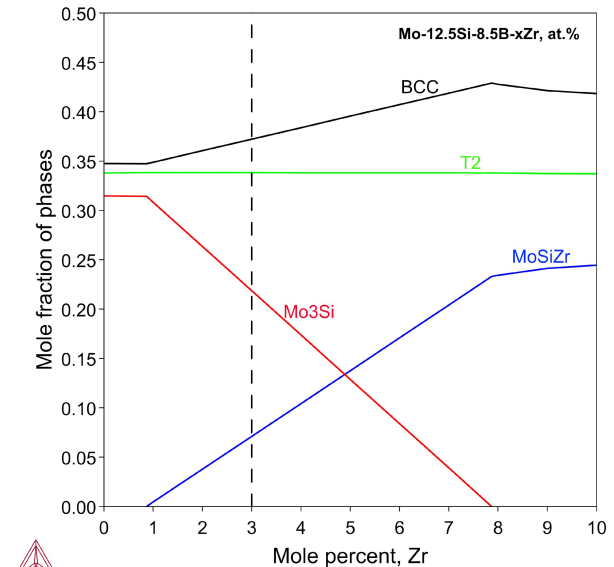
TCS Mo-based Alloys Database (TCMO1)

Example: Mo-Si-B based Alloys

Phase fractions of Mo-12.5Si-8.5B-xTi(Zr) alloys and phase compositions of Mo-12.5Si-8.5B-27.5Ti alloy at 1600 °C



		Exp.	Calc. [TCMO1]
BCC	x(Mo)	0.695	0.735
	x(Ti)	0.245	0.241
	x(Si)	0.023	0.023
Mo3Si	x(Mo)	0.477	0.478
	x(Ti)	0.299	0.272
	x(Si)	0.224	0.25
	x(B)	~0	0
T2	x(Mo)	0.35	0.361
	x(Ti)	0.29	0.264
	x(Si)	0.135	0.125
	x(B)	0.225	0.25
T1	x(Mo)	0.246	0.231
	x(Ti)	0.387	0.394
	x(Si)	0.367	0.375
	x(B)	~0	0



[1] Y. Yang, H. Bei, S.L. Chen, E.P. George, J. Tiley, Y.A. Chang. Effects of Ti, Zr, and Hf on the phase stability of Mo_{ss}+Mo3Si+Mo5SiB2 alloys at 1600°C. Acta Materialia 58 (2010) 541-548.

TCS Nb-based Alloys Database (TCNB1)

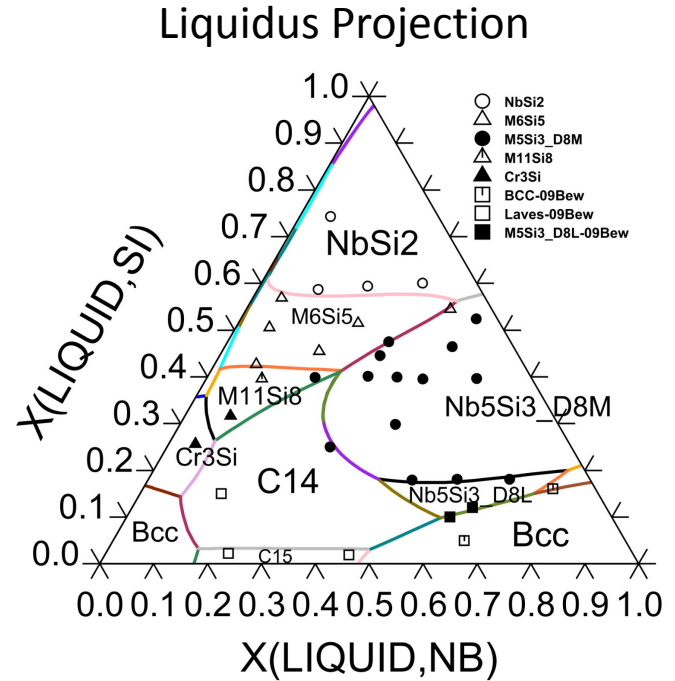
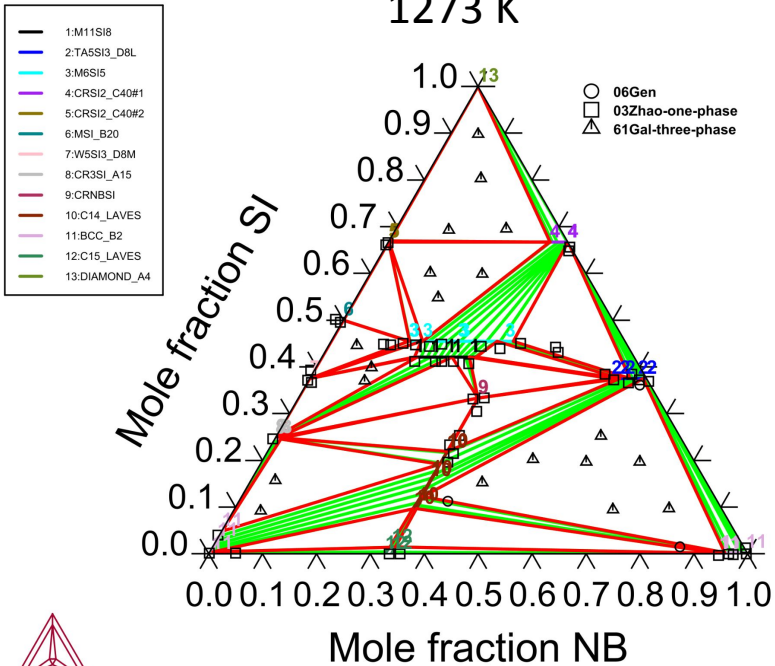
- 12 elements: Al-C-Cr-Hf-Mo-**Nb**-Si-Ta-Ti-V-W-Zr
- All (66) binaries assessed within the framework.
- 76 ternary systems (36 Nb-related) assessed.

Nb-Al-Cr	Nb-Al-Mo	Nb-Al-Si	Nb-Al-Ti	Nb-Al-V	Nb-Al-W	Nb-C-Cr	Nb-C-Hf
Nb-C-Mo	Nb-C-Ta	Nb-C-Ti	Nb-C-V	Nb-C-W	Nb-C-Zr	Nb-Cr-Hf	Nb-Cr-Mo
Nb-Cr-Si	Nb-Cr-Ta	Nb-Cr-Ti	Nb-Cr-V	Nb-Cr-W	Nb-Cr-Zr	Nb-Hf-Si	Nb-Hf-Ti
Nb-Mo-Si	Nb-Mo-Ta	Nb-Mo-V	Nb-Si-Zr	Nb-Si-Ta	Nb-Si-Ti	Nb-Si-V	Nb-Si-W
Nb-Si-Zr	Nb-Ta-Ti	Nb-Ti-V	Nb-V-Zr				

- 101 phases included

TCS Nb-based Alloys Database (TCNB1)

Cr-Nb-Si

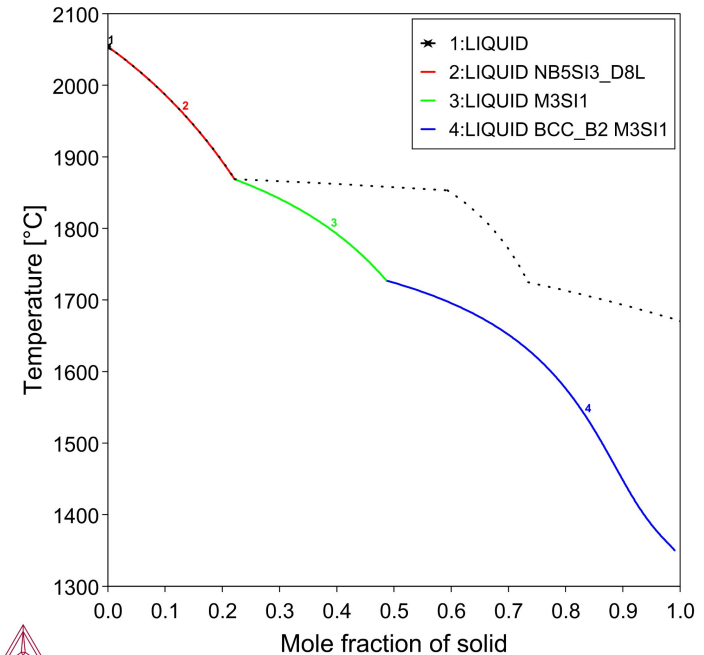


TCS Nb-based Alloys Database (TCNB1)

Comparison between the phases observed from as-cast Nb-Hf-Si-Ti alloys [2007Yang] and those predicted from Scheil simulation.

Alloy Composition	Phases Observed From As-cast Alloys	Phases Predicted From Scheil Simulation
Nb-7.5Hf-21Ti-16Si	Bcc, M3Si	Bcc, M3Si
Nb-12.5Hf-21Ti-16Si	Bcc, M3Si	Bcc, M3Si
Nb-10Hf-33Ti-16Si	Bcc, M3Si, M5Si3	Bcc, M3Si, M5Si3
Nb-8Hf-25Ti-22Si	Bcc, M3Si, Nb5Si3	Bcc, M3Si, Nb5Si3

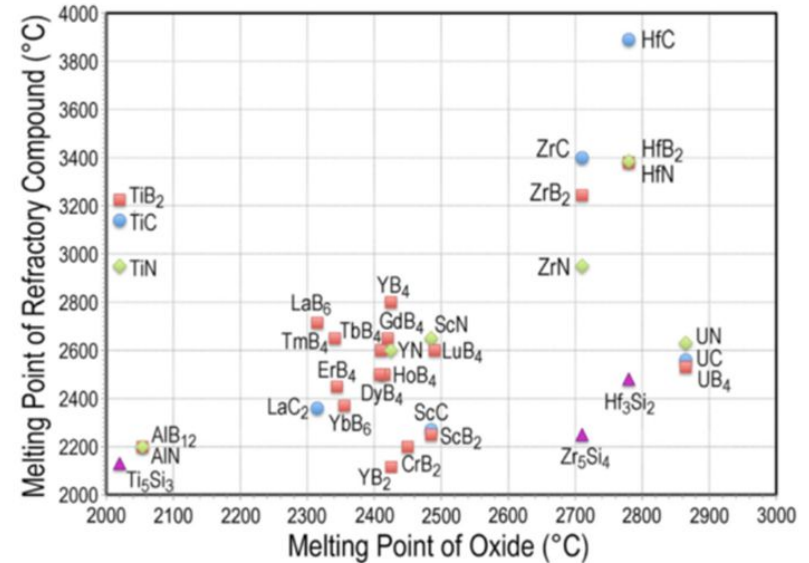
Y. Yang et al., J. Phase Equilibria and Diffusion, 28 (2007) 107-114



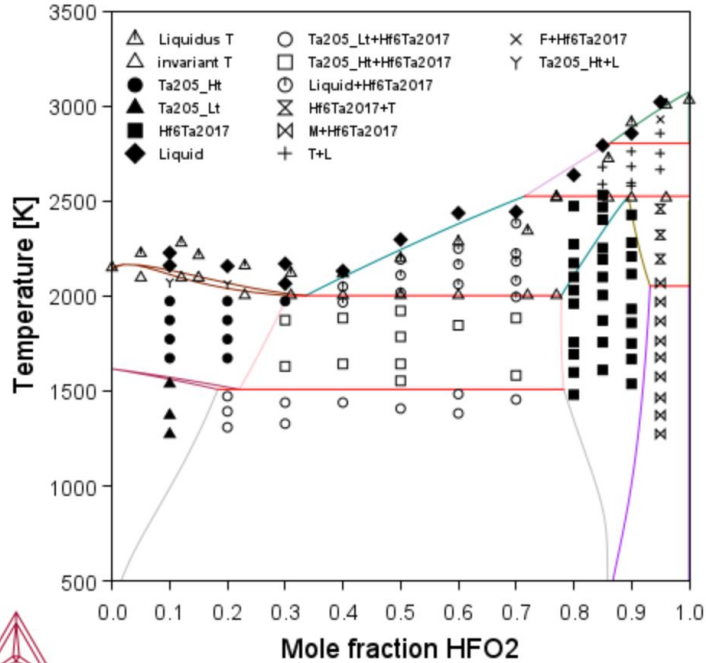
Calculated solidification path of Nb-8Hf-25Ti-22Si using the Scheil and equilibrium model

TCS Ultra-high Temperature Materials Database (TCUHTM2)

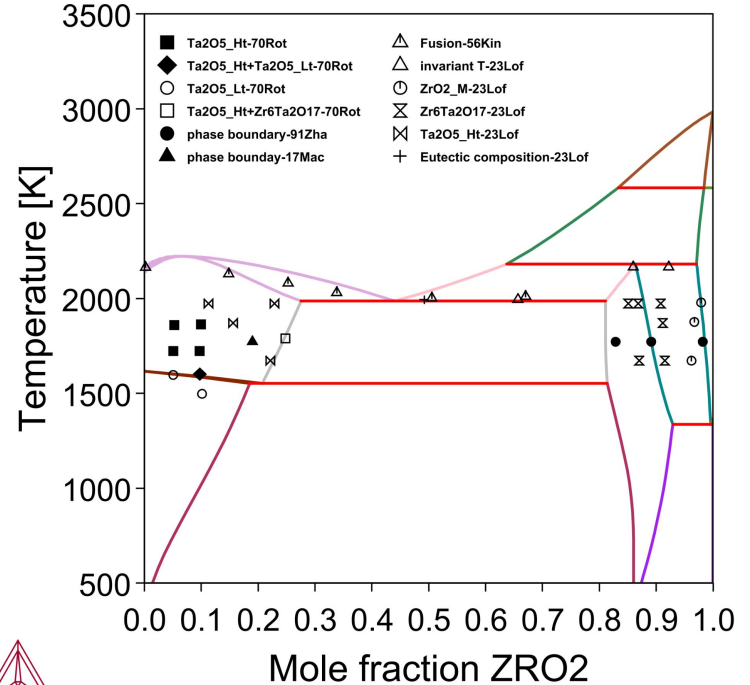
- Add one new element, O. Now it is an 8 elements framework: B-C-Hf-N-O-Si-Ta-Zr.
- 47 phases are included. Ionic liquid model was used for the liquid solution phase.
- 28 binary systems are included. 7 O-X binary systems are assessed.
- 41 ternary system are included. 15 oxygen related ternary systems were assessed and added: **B-Hf-O (T)**, **B-N-O (T)**, **B-O-Si**, **B-O-Zr**, **C-Hf-O (T)**, **C-O-Zr**, **Hf-O-Si**, **Hf-O-Zr**, **O-N-Si**, **O-Si-Zr**, **Hf-N-O**, **Hf-O-Ta**, **N-O-Zr**, **O-Si-Ta**, and **O-Ta-Zr**



TCS Ultra-high Temperature Materials Database (TCUHTM2)



Ta₂O₅-HfO₂



Ta₂O₅-ZrO₂

TCS Ti/TiAl-based Alloys Database (TCTI6)

Thermodynamic Assessments

- **Ti-Ni** improved with the modelling of metastable phases, B19_PRIME, B19_ORTHO, R_MARTE, Ti₂Ni₃, Ti₃Ni₄
- **8 ternaries** (Ti-Al-Ni, Ti-Al-Ta, Ti-B-Ni, Ti-Cr-Fe, Ti-Cu-Ni, Ti-H-Ni, Ti-Ni-Pd, Ti-Ni-Sn), **2 binaries** (Mn-W, O-Sn) updated
- Full gas descriptions updated

Elastic Properties for Ti-based Alloys Available

- Elastic constants (C₁₁, C₁₂, C₁₃, C₃₃, C₄₄) for HCP, BCC, FCC phases
- Elastic moduli (bulk/shear/Young's modulus)

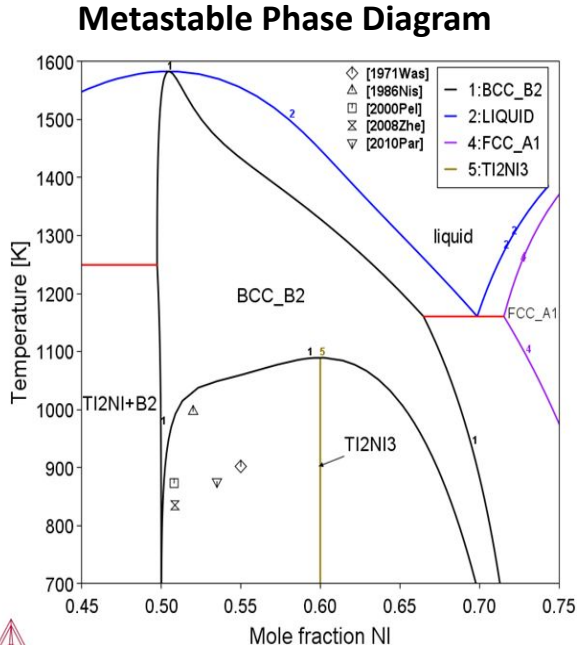
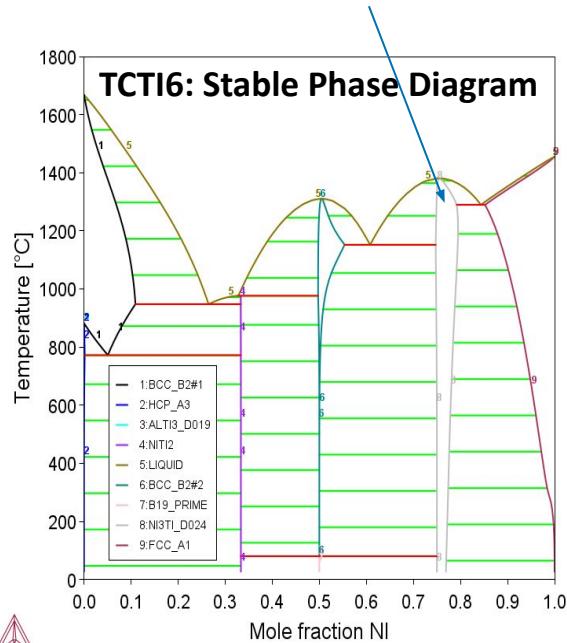
Other Updates

- Surface tension of Fe-Ni
- Molar volume of Bcc_A2 in Al-V, Nb-Ti, Ta-Ti, Al-Ti-V, Ti-V-Zr

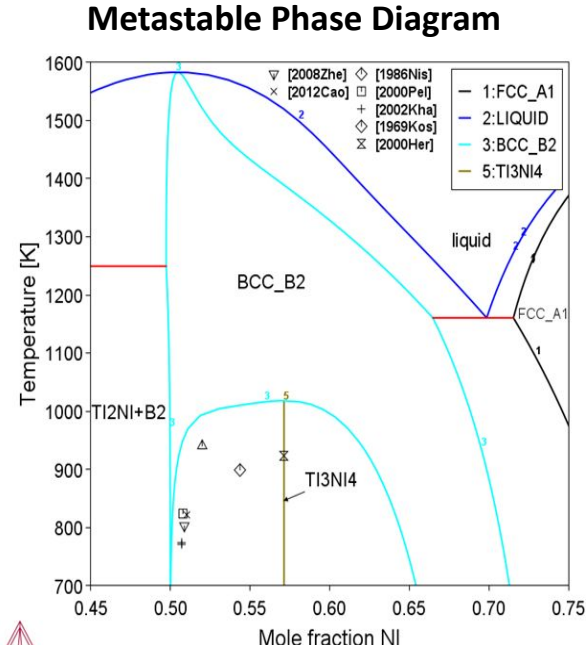
TCS Ti/TiAl-based Alloys Database (TCTI6)

Ti-Ni: Metastable Phases Ti₂Ni₃, Ti₃Ni₄

Experimental studies on Ti-52Ni alloy found Ti₃Ni₄, Ti₂Ni₃, TiNi₃ phases. Phase transformations occur in the following order with increasing aging temperature and time,



Symbols denote conditions of experimentally observed B2+Ti₂Ni₃



Symbols denote conditions of experimentally observed B2+Ti₃Ni₄

TCS Ti/TiAl-based Alloys Database (TCTI6): Elastic Properties

- Elastic constants of TCTI6 elements and systems have been assessed and are available for FCC, BCC and HCP phases.
 - For cubic (FCC, BCC) phases the independent elastic constants are C_{11} , C_{12} and C_{44} .
 - For hexagonal (HCP) phase the independent elastic constants are C_{11} , C_{12} , C_{13} , C_{33} and C_{44} .
- The assessed elastic constants are used to derive the polycrystalline elastic moduli (bulk, shear and Young's) using the Voigt-Reuss-Hill averaging method. They are expressed in terms of the Voigt (upper limit) and Reuss (lower limit) estimates of the elastic moduli:

Bulk modulus

$$B = \frac{1}{2}(B_V + B_R)$$

Shear modulus

$$G = \frac{1}{2}(G_V + G_R)$$

Young's modulus

$$E = \frac{9BG}{3B + G}$$

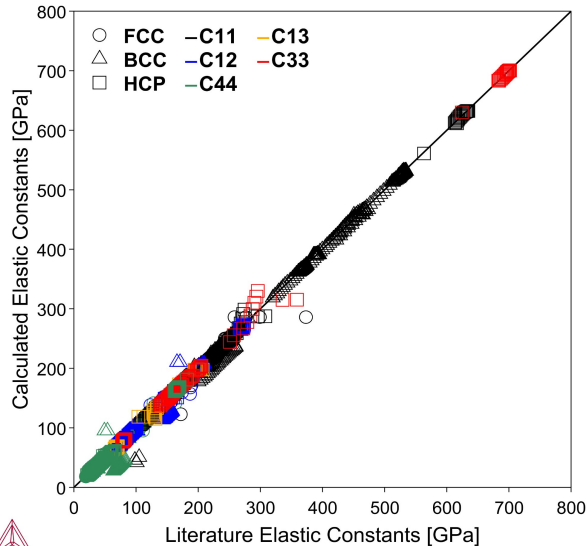
- The Voigt and Reuss estimates depend on crystal symmetry. For cubic (FCC, BCC) solids they are:

$$B_V = B_R = \frac{1}{3}(C_{11} + 2C_{12}) \quad G_V = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}) \quad G_R = \frac{5(C_{11} - C_{12})C_{44}}{3(C_{11} - C_{12}) + 4C_{44}}$$

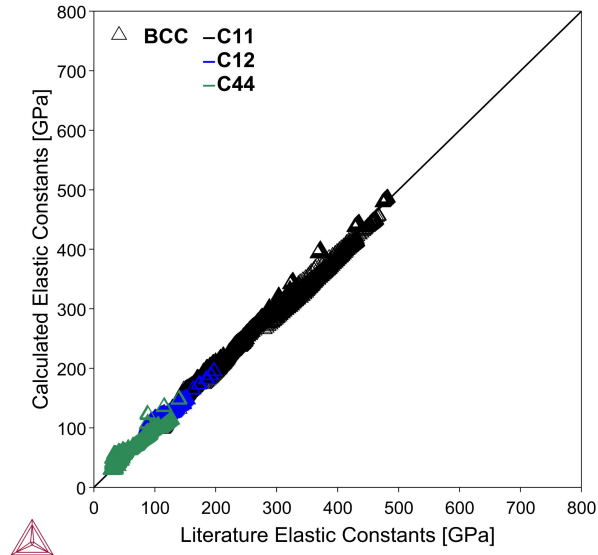
TCS Ti/TiAl-based Alloys Database (TCTI6): Elastic Properties

Example: Literature vs Calculated Elastic Constants

TCTI unaries in different phases at different temperatures.



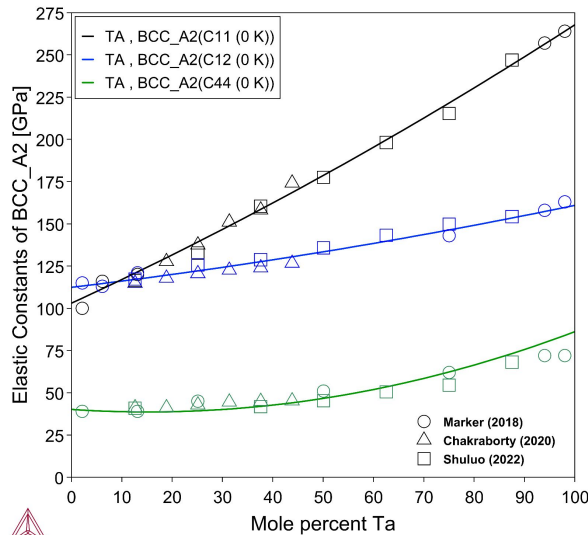
TCTI titanium binaries and other important binary systems for titanium alloys in BCC phase at different temperatures and compositions



TCS Ti/TiAl-based Alloys Database (TCTI6): Elastic Properties

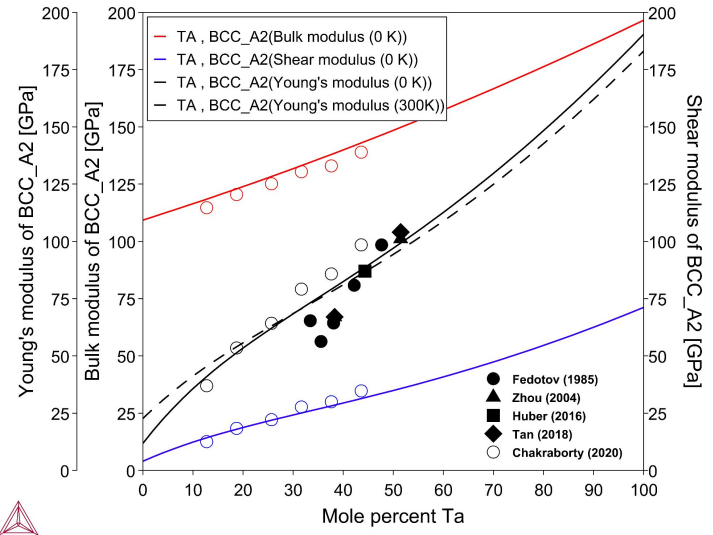
Example: Elastic Moduli of BCC Ti-Ta Alloys

C11
C12
C44



DFT calculations (open symbols)

Bulk
Young's
Shear



DFT calculations (open symbols)
Room temperature experiments (filled symbols)

TCS Solder Alloy Solutions Database (TCSLD5)

- Focused on **brazing alloys**
- 24 elements (new elements are in green):

Ag	Al	Au	Bi	Ca	Cd	Co	Cu	Ga	Ge	Hf	In
Mg	Mn	Ni	Pb	Pd	Pt	Sb	Si	Sn	Ti	Zn	Zr

- 161 assessed binary systems:
 - **19 new** binary systems (green) and **3 reassessed** binary systems (blue):

Ag-Hf	Ag-Ti	Ag-Zr	Bi-Mg	Bi-Mn	Cu-Hf	Cu-Ti	Cu-Zr	Ga-Hf	Ga-Ti	Ga-Zr
Hf-Sn	Hf-Ti	Hf-Zr	In-Pb	In-Ti	In-Zr	Mg-Pb	Ni-Pb	Sn-Ti	Sn-Zr	Ti-Zr

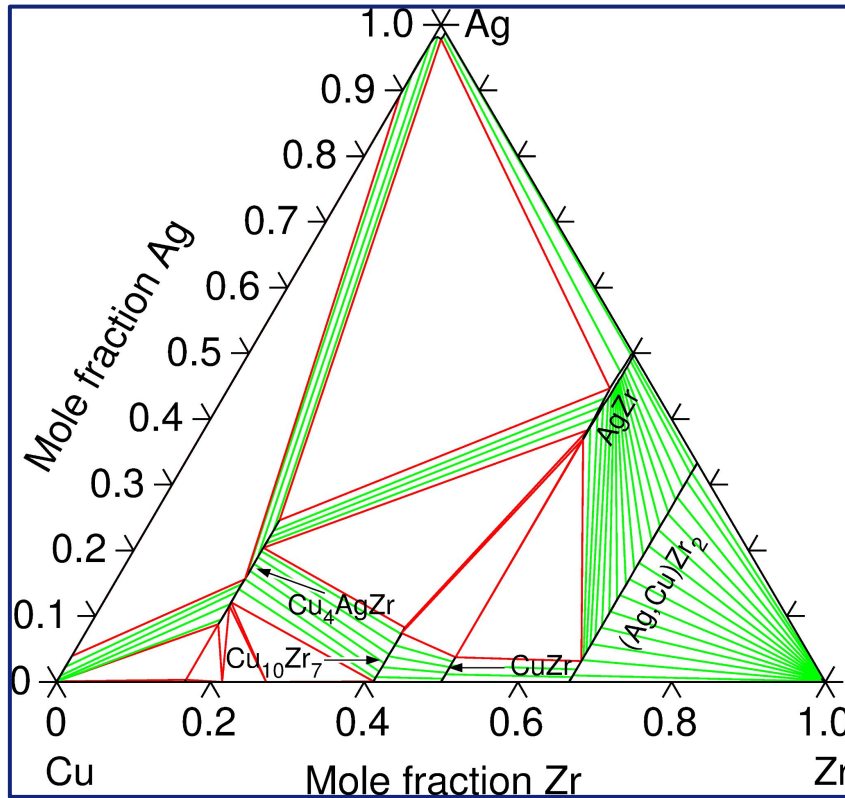
- 77 assessed ternary systems:
 - **5 new** ternary systems (green) and **1 reassessed** ternary system (blue)

Ag-Cu-Ga	Ag-Cu-Ti	Ag-Cu-Zr	Bi-Sb-Sn	Cu-Sn-Ti	Cu-Ti-Zr
----------	----------	----------	----------	----------	----------

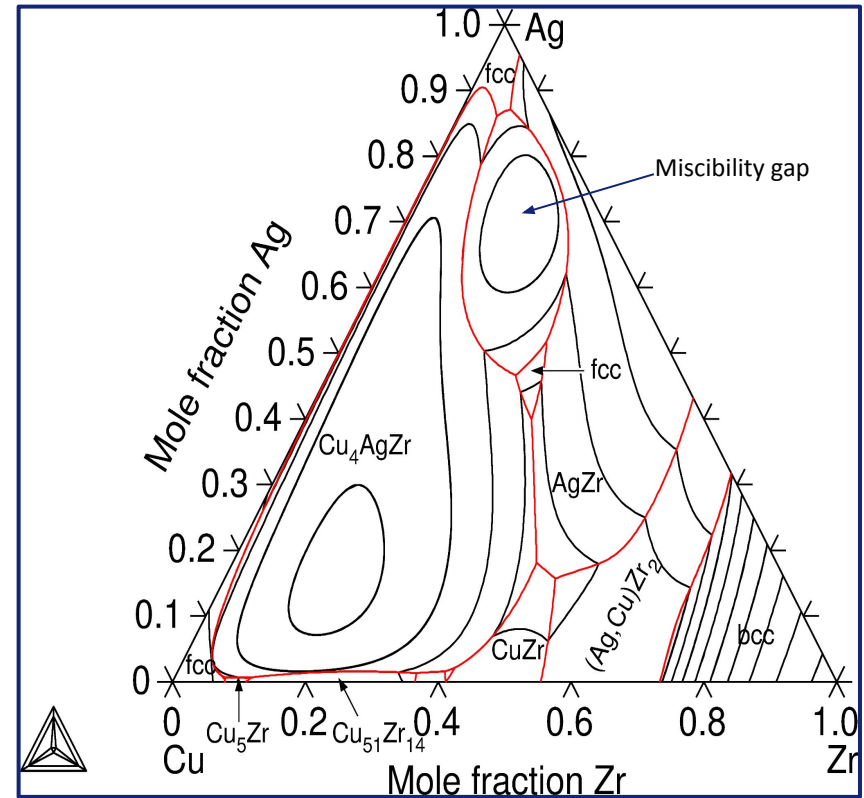
- 328 phases (56 new)
- The HCP_A3 phase restored to describe the lattice stability of Zn (HCP_ZN removed)

TCS Solder Alloy Solutions Database (TCSLD5)

Ag-Cu-Zr: Isothermal Section at 750 °C



Ag-Cu-Zr: Liquidus Surface



TCS Mo-based Alloys Mobility Database (MOBMO1)

1 Elements (12)

Al, B, C, Cr, Fe, Hf, Mn, Mo, Re, Si, Ti, Zr

2 Phases (10)

Solution phases (5)

FCC_A1, BCC_A2, BCC_B2, HCP_A3, LIQUID

Compounds (5)

MO5SI3_D8M, MO3SI_A15, MOSI2_C11B,
C15_LAVES, M6C

3 Included Systems

27 binary- and 8 ternary- systems for solid phases are assessed.

Parameters for self- and impurity- diffusivity of all the liquid systems are estimated using the Modified Sutherland equation. (66 systems)

TCS Mo-based Alloys Mobility Database (MOBMO1)


 Assessed systems

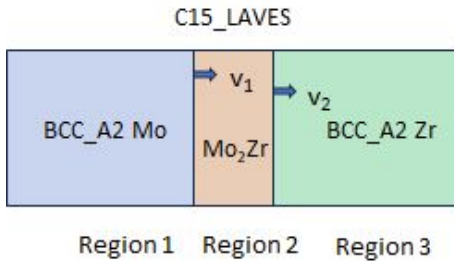
(having interaction parameters)

**MOBMO1**

FCC_A1(9)	BCC_A2(23)	HCP_A3(3)	Compounds
Al-Cr, Al-Fe, Al-Si, Al-Ti, Cr-Fe, Fe-Si, Fe-Mn, Fe-Mn-Si, Fe-Cr-C	Al-Fe, Al-Ti, Cr-Fe, Cr-Mo, Cr-Ti, Fe-Mn, Fe-Mo, Fe-Si, Fe-Ti, Hf-Mo, Hf-Ti, Hf-Zr, Mn-Ti, Mn-Zr, Mo-Ti, Mo-Zr, Zr-Ti, Fe-Cr-Mo, Fe-Mn-Si, Ti-Al-Cr, Ti-Al-Fe, Ti-Al-Mo, Ti-Al-Zr	C-Mo, Cr-Fe, Fe-Zr	MO5SI3_D8M: Mo_5Si_3 C15_LAVES: ZrMo_2 M6C: $\text{Fe}_3\text{Mo}_2\text{C}$

TCS Mo-based Alloys Mobility Database (MOBMO1)

Moving boundary problems:
(Diffusion in multi-phases)

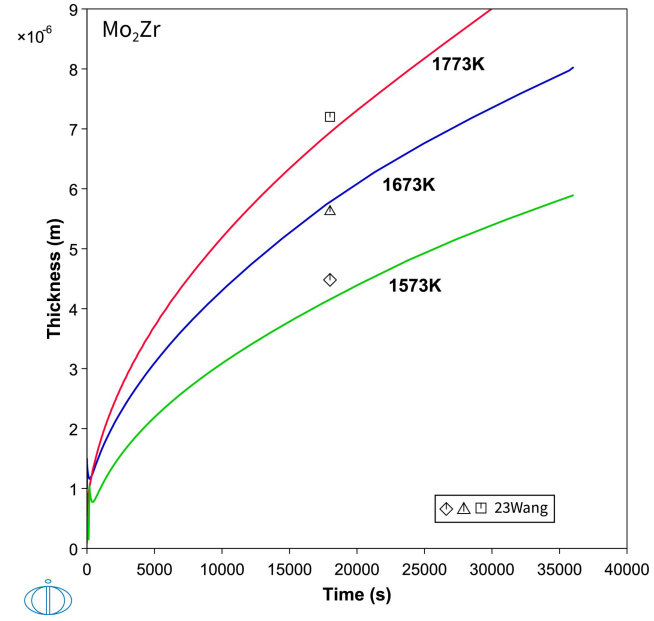
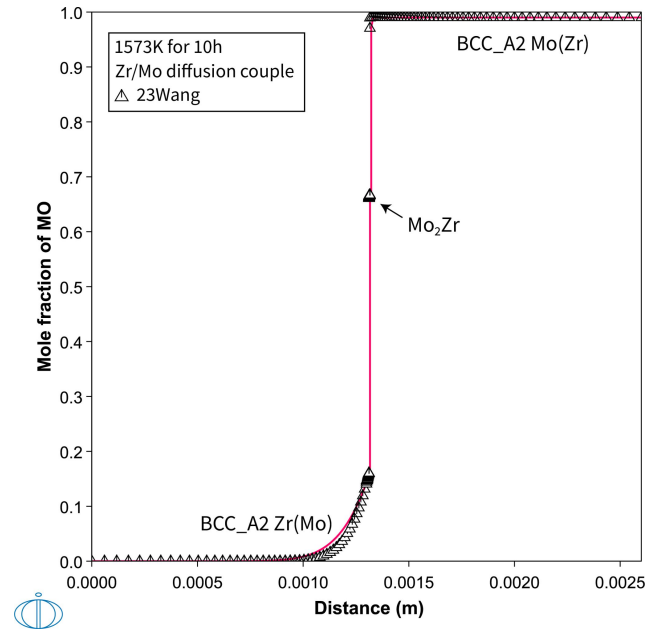


Diffusion couple:

Mo/Mo₂Zr/Zr

Temperature: 1573-1773K

Annealing time: 36000s



TCS Nb-based Alloys Mobility Database (MOBNB1)



Introduction

MOBNB1 is a kinetic database containing atomic mobility data for Nb-based refractory alloys for diffusion-controlled phenomena using the Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA).

MOBNB1 is compatible and primarily recommended for use with TCNB1 thermodynamic database.

1 Elements (12)

Al, C, Cr, Hf, Mo, Nb, Si, Ta, Ti, V, W, Zr

2 Phases (6)

Solution Phases (4)

BCC_A2 FCC_A1 HCP_A3 LIQUID

Compounds (2)

CRS12_C40, NB5SI3_D8L

TCS Nb-based Alloys Mobility Database (MOBNB1)


 Assessed systems

(having interaction parameters)

**MOBNB1**

BCC_A2 (38)	FCC_A1	HCP_A3 (2)	Compounds (2)
Al-Nb, Al-Ti, Al-V, Cr-Nb, Cr-Ta, Cr-Ti, Hf-Nb, Hf-Ta, Hf-Ti, Mo-Cr, Mo-Hf, Mo-Nb, Mo-Ta, Mo-Ti, Mo-W, Nb-Ta, Nb-Ti, Nb-V, Nb-W, Ta-Ti, Ta-W, Ti-V, Zr-Hf, Zr-Mo, Zr-Nb, Zr-Ta, Zr-Ti, Zr-V, Ti-Al-Nb, Ti-Cr-Nb, Ti-Nb-Ta, Ti-Nb-V, Zr-Ta-Nb, Zr-Ti-Nb, Ti-Nb-Ta-Zr, Ti-Nb-Hf-Zr, Ti-Nb-Zr-W, Ti-Cr-Nb-Zr	Al-Si, C-Nb	C-Mo, C-Nb	CRS12_C40: NbSi ₂ NB5SI3_D8L: Nb ₅ Si ₃

TCS Ti-alloys Mobility Database (MOBTI5)

1 Elements (28)

Ag, Al, B, C, Co, Cr, Cu, Fe, H, Hf, Mn, Mo, N, Nb, Ni, O, Pd, Pt, Re, Ru, Si, Sn, Ta, Ti, V, W, Y, Zr

2 Phases (5)

Solution Phases (3)

BCC_A2 HCP_A3 LIQUID

Compounds (2)

Ti3Al (ALT13_D019), TiAl (ALTI_L10)



3 Included Systems

46 binary- and 28 ternary/quaternary- systems for solid solution phases, 14 elements in ALTI_L10 compound, and 6 elements in the ALT13_D019 compound are assessed.

Parameters for self- and impurity- diffusivity of all the liquid systems are estimated using the Modified Sutherland equation. (378 binary systems)

TCS Ti-alloys Mobility Database (MOBTI5)

❖ DICTRA simulations

Diffusion-controlled simulations in multi-component systems:

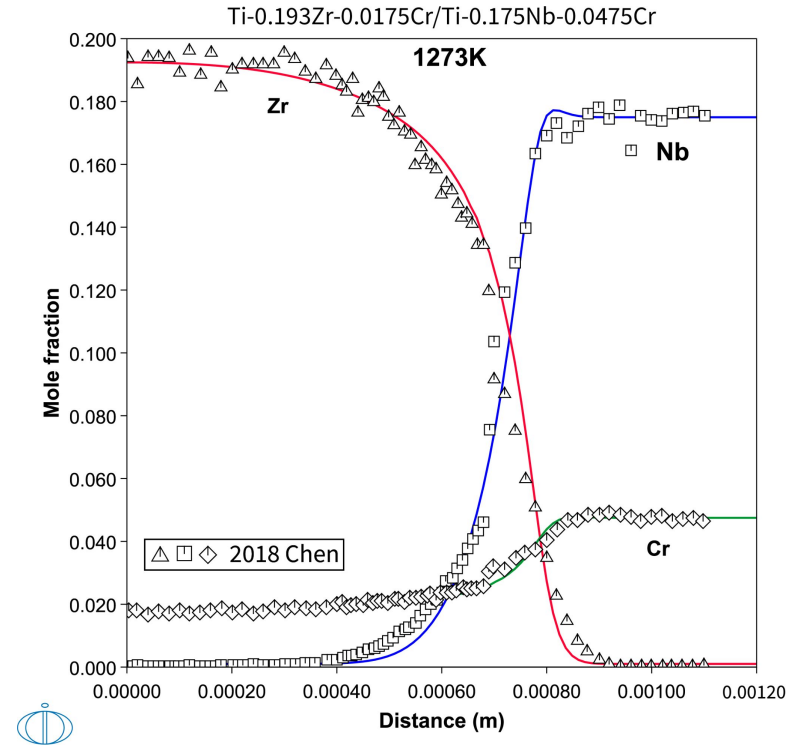
Diffusion in single phase

Diffusion couple: (mole fraction)

Temperature: 1273K

Annealing time: 90000s

The plots show the homogenization results from the DICTRA simulations. The simulations were performed by using the MOBTI5 combined with the TCTI6.



TCS Solder Alloy Solutions Mobility Database (MOBSLD2)



Introduction

MOBSLD2 is a kinetic database containing atomic mobility data for solder alloys for diffusion-controlled phenomena using the Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA).

MOBSLD2 is compatible and primarily recommended for use with TCSLD5 thermodynamic database.

1 Elements (24)

Ag, Al, Au, Bi, Ca, Cd, Co, Cu, Ga, Ge, In, Mg, Mn, Ni, Pb, Pd, Pt, Sb, Si, Sn, Zn, Hf, Ti, Zr (new)

2 Phases (12)

Solution Phases (6)

FCC_A1, HCP_A3, BCT_A5, DIAMOND_A4, RHOMBOHEDRAL_A7, LIQUID

Compounds (Updated: 6)

NI3SN4, CU2IN_LT, CU7IN3, ALCU_ZETA, CU5ZN8_GAMMA, CU3SN

TCS Solder Alloy Solutions Mobility Database (MOBSLD2)


 Assessed systems

(having interaction parameters)



FCC_A1	HCP_A3	Compounds	Other Phases
<p>Binary: ...(29 systems from MOBSLD1)...</p> <p>Updated: Ag-Ge, Ag-Mg, Ag-Mn, Ag-Pd, Al-Pt, Al-Ti, Al-Zr, Au-Pt, Co-Mn, Co-Ti, Cu-Ge, Ni-Pd, Ni-Ti and Pd-Pt</p> <p>Ternary/Quaternary: ...(16 systems from MOBSLD1)...</p> <p>Updated: Ag-Cu-Ni, Ag-Sn-Zn, Cu-Sn-Zn, Cu-Ni-Sn, Cu-Al-Ni and Cu-Al-Sn.</p>	<p>Updated: Ag-Mg, Ag-Ti, Cu-Ti, Mg-Ga, Mg-Zn and Mg-Ag-Zn</p>	<p>NI3SN4: Cu, Ni, In, Sn CU2IN_LT: Cu, In CU7IN3: Cu, In, Sn CU11IN9: Ag, Cu, Al, In CU5ZN8: Au, Ni, Sn, Zn CU3SN: other elements</p>	<p>Add self- and impurity-diffusivity data for Hf-X, Ti-X and Zr-X binary systems</p>

TCS Aluminum-based Alloys Database (TCAL9 to Version 9.1)

- Thermal conductivity and electrical resistivity of liquid Al were re-assessed.
- Electrical resistivity of the liquid phase in the Al-Si system was re-assessed.
- Surface tension parameters were updated for the systems Ag-Cu, Bi-Sn, Cu-Sn, and Ag-Cu-Sn.
- Viscosity parameters were updated for the systems Ag-Cu, Al-Sb, Al-Te, B-Bi, B-Mg, B-Pb, B-Sn, B-Sr, B-Zn, Bi-C, Bi-Fe, Bi-Mo, Bi-Nd, C-Ca, C-Pb, C-Sn, Cr-Pb, Mg-Sb, Mg-Sn, Mo-Pb, Mo-Sn, Nb-Pb, Pb-Ti, Pb-V, and Cu-Ti-Zr.
- The FCC_A1 parameters were corrected in the Cu-Hf system.

Thermophysical Properties

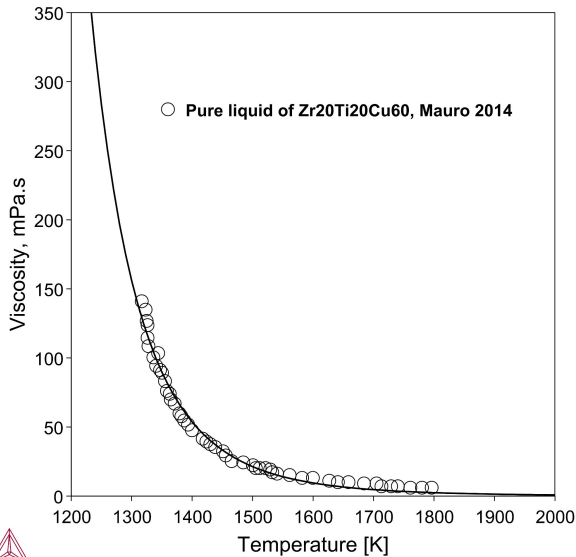
	TCMO1	TCSLD5	TCNB1	TCUHTM2	TCTI6 *	TCAL9.1
Molar Volume	X	X	X	X	X	X
Surface Tension	X	X	X		X	X
Viscosity	X	X	X		X	X
Thermal Conductivity	X	X	X		X	X
Electrical Resistivity	X	X	X		X	X

* TCTI6

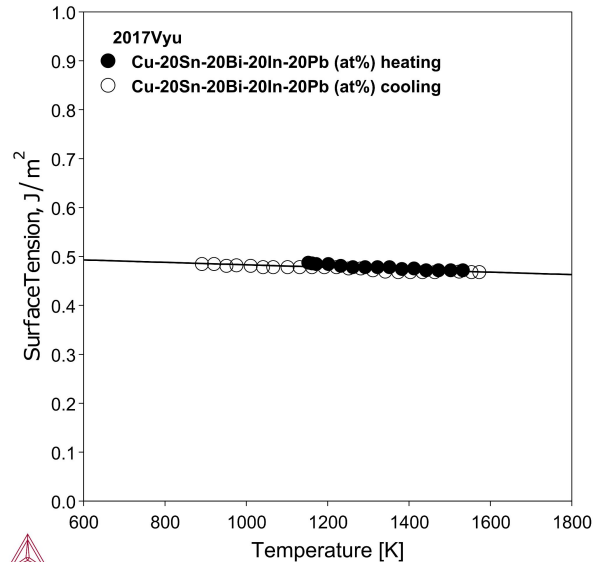
- Improved surface tension of Fe-Ni.
- Molar volumes of BCC_A2 phase are revised for the systems Al-V, Nb-Ti, Ta-Ti, Al-Ti-V, and Ti-V-Zr.

Thermophysical Properties: Examples

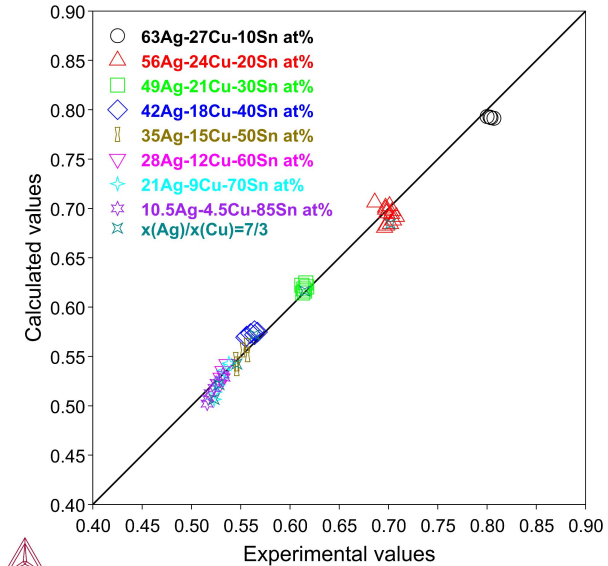
Viscosity Cu-Ti-Zr, TCSLD5



Surface Tension Cu-Sn-Bi-In-Pb, TCSLD5



Surface Tension Ag-Cu-Sn, TCSLD5/TCAL9.1



Thank You for Attending the Webinar!

AM Module Highlights

- ✓ Keyhole model with fluid flow
- ✓ Printability maps in Graphical mode

Property Model Highlights

- ✓ New Titanium Model Library
- ✓ Parallelization of property model calculator
- ✓ Martensitic Steel Strength Property Model improvements

Database Highlights

- ✓ Two new Refractory alloy databases TCMO1 and TCNB1, come paired with kinetic databases
- ✓ Oxygen added to TCUHTM2 Ultra-High Temperature Materials database
- ✓ TCTI6 Titanium alloy database with Elastic constants
- ✓ Brazing elements added to TCSLD5 solder database

Q & A

- Please type questions into the Q&A feature
- Or “raise your hand” to ask to be unmuted

Do you want a free consultation of the software applied to your work?

Contact us at info@thermocalc.com

Or visit our website www.thermocalc.com for more information