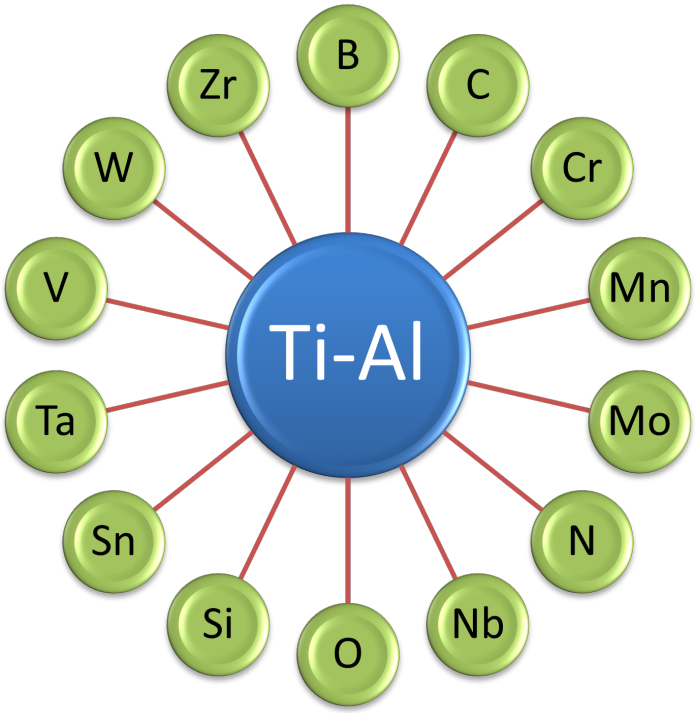
Pandat 2025

Database Manual

CompuTherm LLC

PanTiAl

Database for multi-component TiAl-based alloys



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Contents

PanTiAl **1**

1 Thermodynamic Database **1**

1.1 Components (16) 1

1.2 Suggested Composition Range 1

1.3 Phases 1

1.4 Key Elements and Subsystems 3

1.5 Database Validation 4

2 Mobility Database **9**

2.1 Phases 9

2.2 Self-diffusivity of Pure Elements 9

2.3 Assessed Systems 10

2.4 Database Validation 10

3 Thermophysical Property Database **12**

3.1 Molar Volume 12

3.2 Surface Tension 13

3.3 Viscosity 14

4 References **15**

PanTiAl2025: List of Phases **1**

1 Thermodynamic Database

1.1 Components (16)

A total of **16** components are included in PanTiAl database as listed here:

Major alloying elements: **Al**, Cr, Mo, Nb, Ta, **Ti**, V, W and Zr

Minor alloying elements: B, C, Mn, N, O, Si and Sn.

1.2 Suggested Composition Range

The suggested composition range for each element is listed in Table 1.1. It should be noted that this given composition range is rather conservative. It is derived from the chemistries of the multicomponent commercial alloys that have been used to validate the current database. In the subsystems, many of these elements can be applied to a much wider composition range. In fact, some subsystems are valid in the entire composition range as given in Section 1.4

Table 1.1: Suggested composition range

Elements	Composition Range (wt.%)
Ti	50-100
Al,Mo,Nb	0-30
Cr,Ta,V,W,Zr	0-10
B, C, N, O, Mn, Si, Sn	0-0.5

1.3 Phases

A total of **208** phases are included in the current database. The names and thermodynamic models of some phases are given in Table 1.2. Information on all the other phases is listed in PanTiAl2025: List of Phases. Users can also view it through TDB viewer of Pandat.

Table 1.2: Phase name and related information

Name	Lattice Size	Constituent
A15	(3)(1)	(Al,Cr,Mo,Nb,Ta,Ti)(Al,Mo,Nb,Sn,Ti)
B2	(1)(1)	(Al,Cr,Mn,Mo,Nb,Ti)(Cr,Mn,Mo,Nb,Ti,Va)
Bcc	(1)(3)	(Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,V,W,Zr) (B,C,N,O,Va)
Bcc_B2	(0.5)(0.5)(3)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,V,W) (Al,Cr,Mn,Mo,Nb,Ta,Ti,V,W)(Va)
D0_19	(0.75)(0.25)(0.5)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,V,Zr) (Al,Mn,Mo,Nb, Sn,Ta,Ti,Zr)(C,O,N,Va)
D0_22	(0.75)(0.25)(0.5)	(Al,Cr,Mo,Si,Ti)(Al,Cr,Mo,Nb,Ta,Ti,V) (C,Va)
Fcc	(1)(1)	(Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,V,W,Zr) (B,C,N,O,Va)
Hcp	(1)(0.5)	(Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,V,W,Zr) (B,C,N,O,Va)
L10_TiAl	(1)(1)(2)	(Al,Cr,Mn,Mo,Nb,Sn,Ta,Ti,V,W,Zr) (Al,Cr,Mn,Mo,Nb,Sn,Ta,Ti,V,W,Zr) (C,O,N,Va)
Laves_C14	(2)(1)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,V,Zr) (Al,Cr,Mn,Mo,Nb,Ta,Ti,V,Zr)
Laves_C15	(2)(1)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,V,W,Zr) (Al,Cr,Mn,Mo,Nb,Ta,Ti,V,W,Zr)
Laves_C36	(2)(1)	(Al,Cr,Ti,V,Zr)(Al,Cr,Ti,V,Zr)
Liquid	(1)	(Al,B,C,Cr,Mn,Mo,N,Nb,O,Si,Sn,Ta,Ti,V,W, Zr,Al2O3,Cr2O3,NbO,NbO2,Nb2O5,SiO2)
Mu	(7)(2)(4)	(Al,Cr,Mn,Mo,Nb)(Mo,Nb,Ti)(Cr,Mo,Nb,Ti)
Sigma	(8)(4)(18)	(Al,Cr,Mn,Ta,W)(Cr,Mo,Nb,Ta,Ti,V,W) (Al,Cr,Mn,Mo,Nb,Ta,Ti,V,W)

1.4 Key Elements and Subsystems

This database is designed for TiAl based alloy applications. A total of **117** subsystems, including 110 binary and 7 ternary subsystems have been assessed. The modeling status is indicated by numbers. The systems with number 10 are fully assessed in the whole composition range. The higher value shows higher reliability of the system.

Binary Systems (110)

Al-B(10)	Al-C(10)	Al-Cr(10)	Al-Mn(10)	Al-Mo(10)	Al-N(8)	Al-Nb(10)
Al-O(10)	Al-Si(10)	Al-Sn(10)	Al-Ta(10)	Al-Ti(10)	Al-V(10)	Al-W(10)
Al-Zr(10)	B-C(10)	B-Cr(10)	B-Mn(10)	B-Mo(10)	B-Nb(10)	B-Si(10)
B-Sn(10)	B-Ta(10)	B-Ti(10)	B-V(10)	B-W(10)	B-Zr(10)	C-Cr(10)
C-Mn(10)	C-Mo(10)	C-Nb(10)	C-Si(10)	C-Ta(10)	C-Ti(10)	C-V(10)
C-W(10)	C-Zr(10)	Cr-Mn(10)	Cr-Mo(10)	Cr-N(10)	Cr-Nb(10)	Cr-O(10)
Cr-Si(10)	Cr-Sn(10)	Cr-Ta(10)	Cr-Ti(10)	Cr-V(10)	Cr-W(10)	Cr-Zr(10)
Mn-Mo(10)	Mn-N(6)	Mn-Nb(10)	Mn-Ni(10)	Mn-O(10)	Mn-Si(10)	Mn-Sn(10)
Mn-Ta(10)	Mn-Ti(10)	Mn-V(10)	Mn-Zr(10)	Mo-N(8)	Mo-Nb(10)	Mo-O(10)
Mo-Si(10)	Mo-Sn(10)	Mo-Ta(10)	Mo-Ti(10)	Mo-V(10)	Mo-Zr(10)	N-Nb(8)
N-Si(8)	N-Sn(8)	N-Ta(8)	N-Ti(8)	N-V(8)	N-Zr(8)	Nb-O(10)
Nb-Si(10)	Nb-Sn(10)	Nb-Ti(10)	Nb-V(10)	Nb-W(10)	Nb-Zr(10)	O-Si(10)
O-Sn(10)	O-Ta(8)	O-Ti(8)	O-V(8)	O-W(10)	O-Zr(10)	Si-Sn(10)
Si-Ta(10)	Si-Ti(10)	Si-V(10)	Si-W(10)	Si-Zr(10)	Sn-Ta(10)	Sn-Ti(10)
Sn-V(10)	Sn-Zr(10)	Ta-Ti(10)	Ta-V(10)	Ta-W(10)	Ta-Zr(10)	Ti-V(10)
Ti-W(10)	Ti-Zr(10)	V-W(10)	V-Zr(10)	W-Zr(10)		

Ternary Systems (7)

Al-Ti-V(10)	Al-Cr-Ti(8)	Al-Mn-Ti(8)	Al-Mo-Ti(8)	Al-Nb-Ti(8)	Al-Si-Ti(8)
Al-Ti-W(8)					

1.5 Database Validation

PanTiAl database focuses on γ-TiAl-based alloys systems. It is very important to get accurate α transus (α→γ) temperatures. Table 1.3 compares the calculated α transus temperatures with the experimental data for various alloys [1992Lom, 1993Fuc, 1995Bho, 1995Fuc, 1995Kim, 2014Pen], which is also shown in Figure 1.1.

Table 1.3: Comparison between the calculated α transus (α→γ) temperatures and experimentally determined ones

Alloys (at.%)	Exp. T (°C)	Calc. T (°C)	Ref.
Ti-48Al-2Cr-2Nb	1364	1366	[1993Fuc]
Ti-47.73Al-1.77Nb-1.99Cr	1366	1360	[1995Fuc]
Ti-46Al-2.5Nb-2.1Cr-0.2B	1330	1321	[1995Bho]
Ti-46.48Al-2.07Nb-2.03Cr	1343	1332	[1995Fuc]
Ti-43Al-6Cr-0.2B	1260	1259	[2014Pen]
Ti-43Al-6Mo-0.2B	1275	1285	[2014Pen]
Ti-43Al-6Nb-0.2B	1255	1257	[2014Pen]
Ti-43Al-2Cr-4Nb-0.2B	1245	1244	[2014Pen]
Ti-43Al-2Mo-4Nb-0.2B	1265	1277	[2014Pen]
Ti-43Al-4Nb-1Cr-1Mo-0.2B	1250	1255	[2014Pen]
Ti-44.81Al-8Nb	1312	1312	[2014Pen]
Ti-45.75Al-8Nb	1352	1337	[2014Pen]
Ti-46.7Al-3Nb-1W	1350	1367	[1995Bho]
Ti-49.5Al-1.1Mn-2.5Nb	1436	1428	[1992Lom]
Ti-47.5Al-1.83Nb-1.86Cr-0.45W	1361	1361	[1995Fuc]

Alloys (at.%)	Exp. T (°C)	Calc. T (°C)	Ref.
Ti-46.57Al-2.02Nb-2.05Cr-0.54W	1359	1339	[1995Fuc]
Ti-47.82Al-1.87Nb-1.98Cr-0.91W	1358	1376	[1995Fuc]
Ti-46.37Al-2.06Nb-2.19Cr-1.04W	1344	1348	[1995Fuc]
Ti-46.5Al-2.1Cr-3Nb-0.2W	1325	1337	[1995Kim]
Ti-47Al-2.6Nb-1Cr-0.9V	1355	1353	[1995Kim]
Ti-47Al-2.3Nb-1.5Cr-0.5V	1362	1349	[1995Kim]
Ti-47Al-2.6Nb-1.5Cr-0.5Mn-0.15B	1365	1356	[1995Kim]

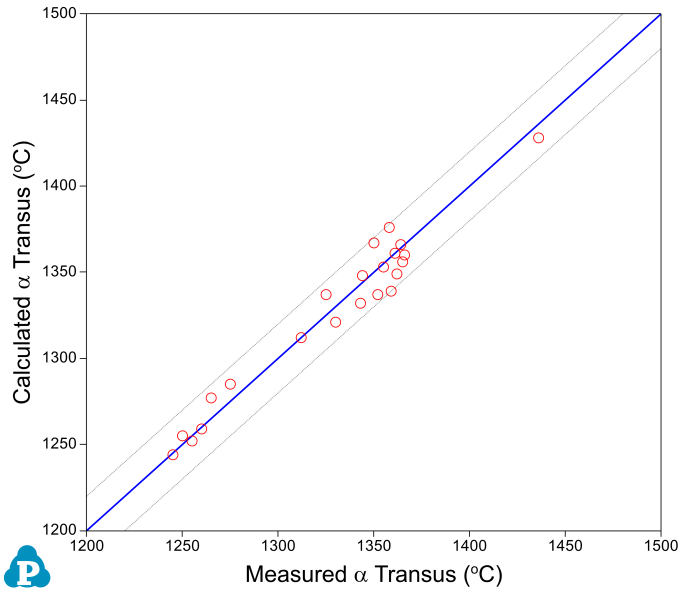

Figure 1.1: Comparison between calculated and measured α transus temperatures [1992Lom, 1993Fuc, 1995Bho, 1995Fuc, 1995Kim, 2014Pen]

Schwaighofer et al. [2014Sch] investigated microstructure and phase evolution of a β-solidifying TNM alloy with a nominal composition of Ti-42.82Al-4.05Nb-1.01Mo-0.11B (in at.%) with minor C and Si (C+Si ≤ 1at.%) by means of uniaxial compressive hot-deformation tests. They carried out in situ high energy X-ray diffraction (HEXRD) experiments to obtain a deeper insight about the deformation behavior of the alloy, i.e. phase fractions and texture

evolution during isothermal and non-isothermal compression. Figure 1.2 shows the comparison between the calculated phase fractions under equilibrium condition and those determined by in situ HEXRD method. The exact contents of C and Si are not mentioned in the reference [2014Sch], so they are not included in the calculation. The calculated results are in reasonable agreement with the experimental data [2014Sch] for the β, α, and γ phases. The α_2 phase starts to form at ~1200 °C, which is higher than 1160 °C for a typical TNM alloy. Considering the stress applied to the sample, the hexagonal based structure of α_2 phase is more favorable than the BCC-based structure of β_0 phase.

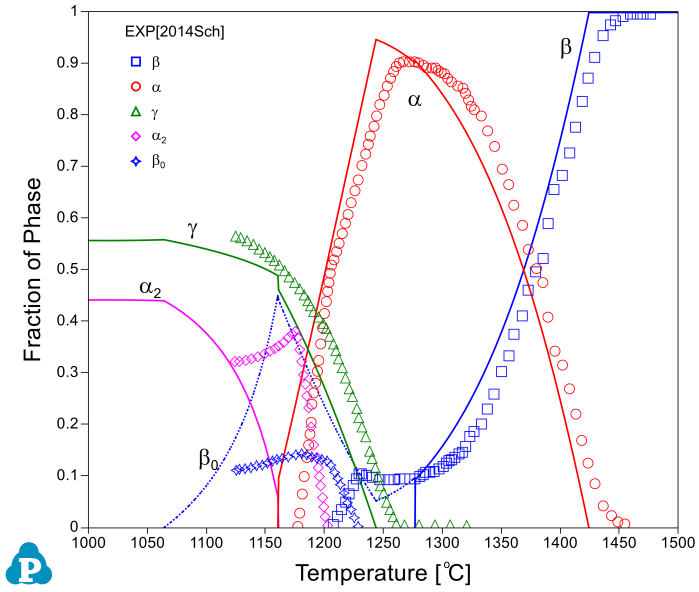

Figure 1.2: Calculated phase fractions for alloy Ti-43Al-4Nb-1Mo-0.1B (in at.%) compared with experimental data [2014Sch]

Kesler [2011Kes] investigated the γ+σ microstructure in the Ti-Al-Nb-Cr-Mo system. The alloy samples were aged at elevated temperatures for 2 hours and then furnace cooled. The volume fractions of the σ phase were obtained by analyzing the SEM-BSE images. The measured fractions are compared with line calculations for these alloys (Ti-45Al-22Nb-5Cr, Ti-45Al-18Nb-5Cr-1Mo, and Ti-45Al-14Nb-5Cr-1Mo), as shown in Figure 1.3, Figure 1.4 and Figure 1.5, respectively. The calculated σ phase fractions slightly increase with

decreasing temperatures while the measured values do not change very much at different temperatures, which may be due to the slow cooling rate after aging. The calculations are in reasonable agreement with the experimental data.

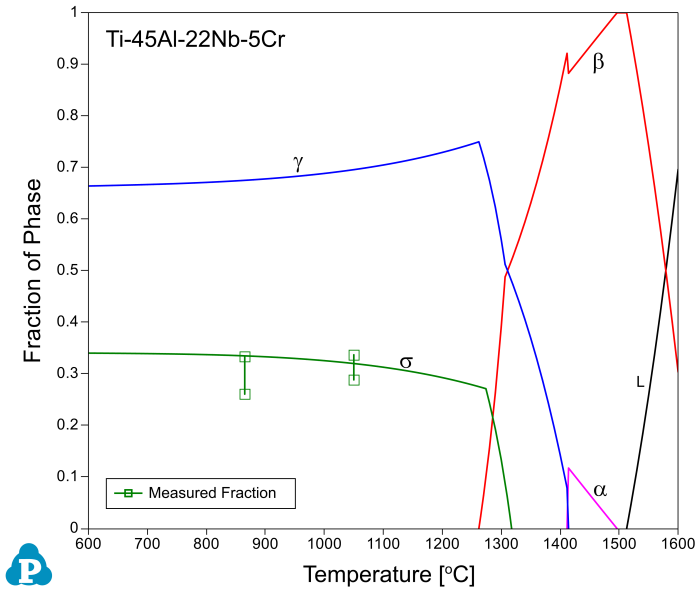

Figure 1.3: Calculated phase fractions for alloy Ti-45Al-22Nb-5Cr (in at.%) compared with experimental data [2011Kes]

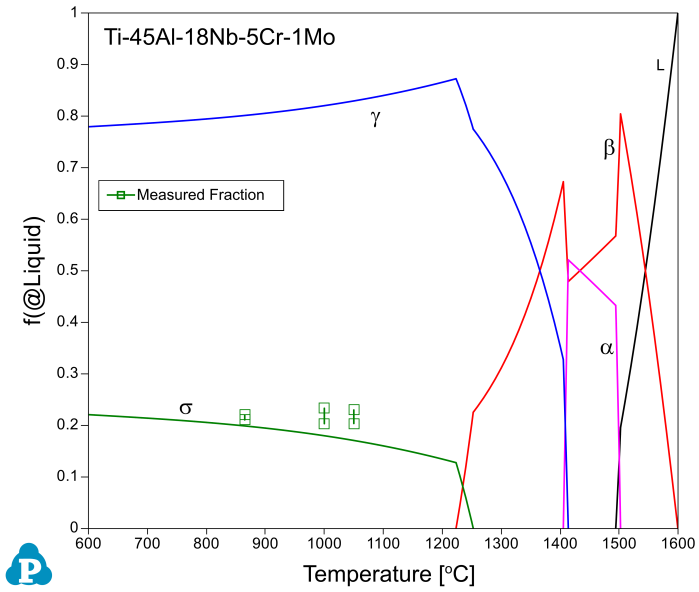

Figure 1.4: Calculated phase fractions for alloy Ti-45Al-18Nb-5Cr-1Mo (in at.%) compared with experimental data [2011Kes]

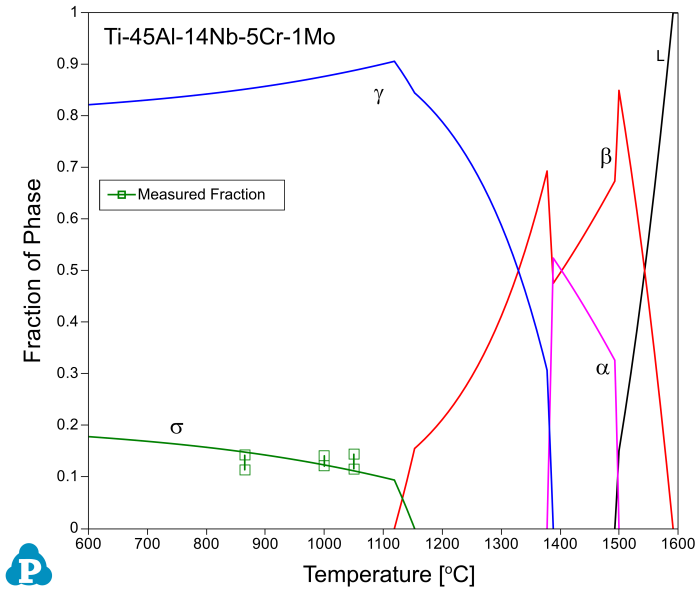

Figure 1.5: Calculated phase fractions for alloy Ti-45Al-14Nb-5Cr-1Mo (in at.%) compared with experimental data [2011Kes]

2 Mobility Database

PanTiAl2025_MB is an atomic mobility database for TiAl-based alloys, which is compatible with the `PanTiAl2025_TH` thermodynamic database and suitable for the simulation of diffusion-controlled phenomena using the **PanDiffusion** module, **PanEvolution** module, and/or **PanSolidification** module.

2.1 Phases

The atomic mobility within the **Liquid**, **Bcc**, **Fcc**, and **Hcp** solution phases are assessed in this database.

2.2 Self-diffusivity of Pure Elements

The self-diffusivity of an element is usually described by an analytical expression. For the stable crystal structures, these expressions can be obtained using the available experimental data, while those for the metastable/unstable states are usually estimated from those of the stable states. In the following tables, we use different color to represent different status:

: Validated

: Estimated

: No data

Table 2.1: Assessed self-diffusivity of pure elements with different crystal structures

	Al	Cr	Mn	Mo	Nb	Si	Sn	Ta	Ti	V	W	Zr
Bcc												
Fcc												
Hcp												

2.3 Assessed Systems

In addition to the assessed self-diffusivities shown above, the impurity diffusion data for all elements included in the current mobility database are also assessed. Moreover, chemical-diffusivities available in some binary and ternary systems are also used to assess the interaction parameters. These binary and ternary systems are listed below for the Bcc phase.

Bcc phase

Al-Ti	Cr-Ti	Mo-Nb	Mo-Ta	Mo-Ti	Mo-W	Nb-Ta	Nb-Ti	Nb-V	Nb-W
Nb-Zr	Ta-Ti	Ta-W	Ti-V	Ti-Zr	V-Zr	Al-Cr-Ti			

2.4 Database Validation

The simulated concentration profiles of a series of Ti-base alloys are shown below to validate the current `PanTiAl2025_MB` database.

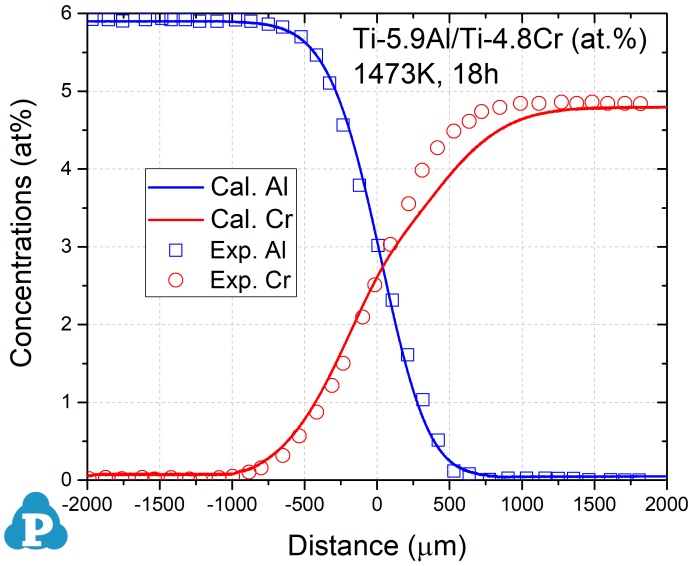

Figure 2.1: Concentration profiles of Ti-5.9Al/Ti-4.8Cr (at.%) at 1473K for 18h [2011Li]

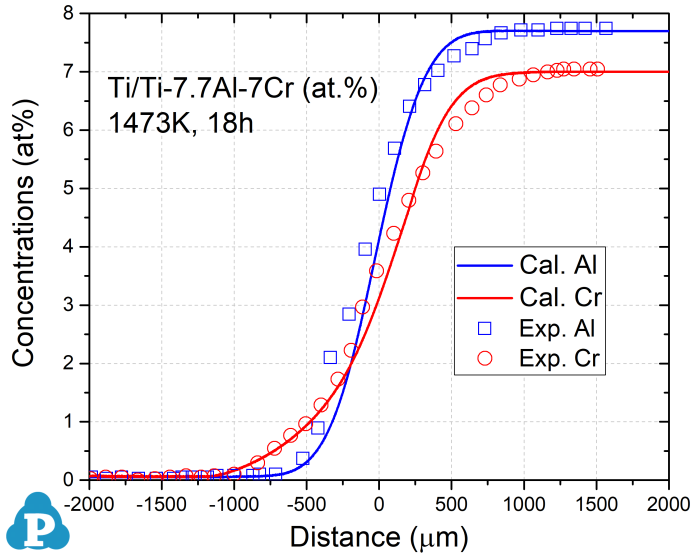

Figure 2.2: Concentration profiles of Ti/Ti-7.7Al-7Cr (at.%) at 1473K for 18h[2011Li]

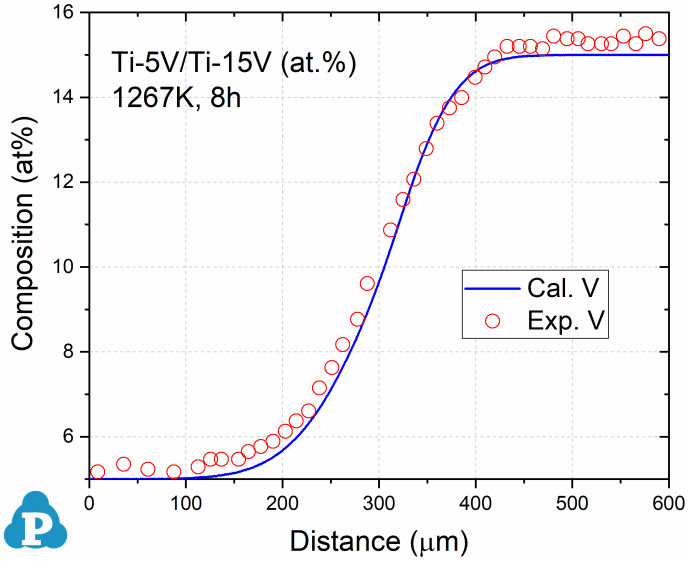

Figure 2.3: Concentration profile of Ti-5V/Ti-15V (at.%) annealed at 1267K for 8h [2009Liu]

3 Thermophysical Property Database

The thermophysical property database **PanTiAl2025_ TP** is compatible with the `PanTiAl2025_ TH` thermodynamic database and suitable for the simulation of thermophysical properties of TiAl-based alloys. It includes the molar volume data for all the phases, surface tension and viscosity properties for the liquid phase.

3.1 Molar Volume

The current molar volume database covers all **208** phases assessed in the `PanTiAl2025_ TH` database. It is used to calculate the density, thermal expansion, solidification shrinkage of the alloys.

The simulated density changes vs. temperature of a series of TiAl-based alloys are shown below to validate the current database.

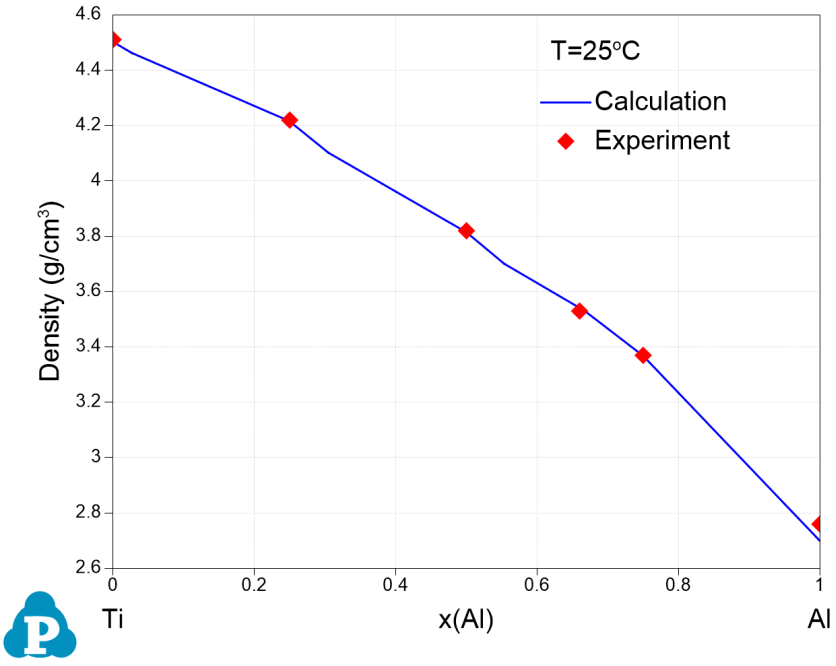

Figure 3.1: Density of Ti-Al binary alloys at 25 °C [1992ASM]

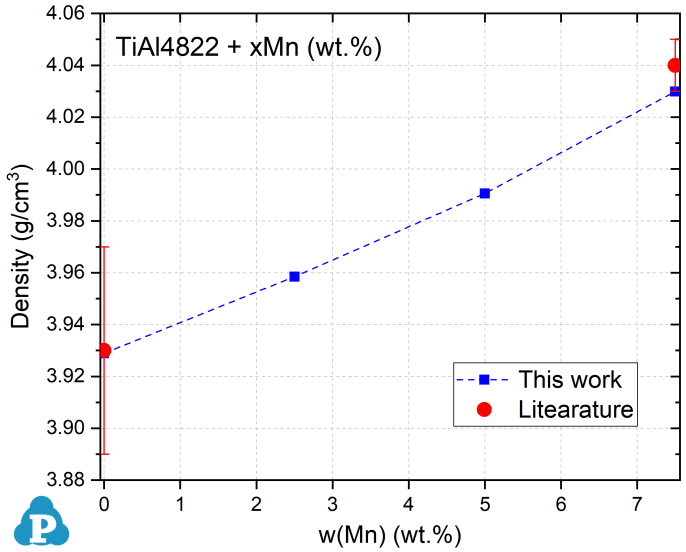

Figure 3.2: Density of TiAl4822+Mn sintered at 1150 °C [2020Ann]

3.2 Surface Tension

The surface tension of the liquid phase is added into the property database. Figure 3.3 shows the surface tension of the TiAl4822 (Ti-34.44Al-2.6Cr-4.7Nb, wt.%) alloy.

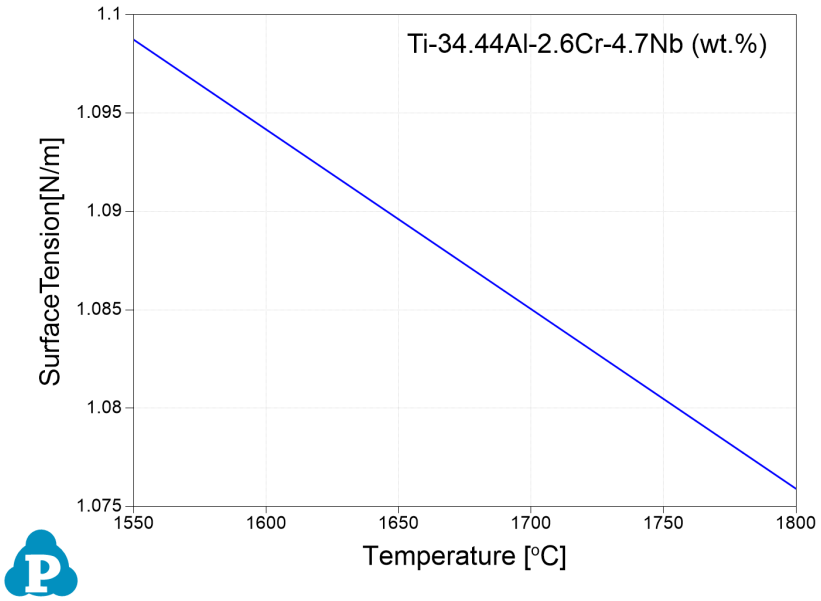

Figure 3.3: Surface tension of the TiAl4822 alloy

3.3 Viscosity

The viscosity of the liquid phase is added into the property database. Figure 3.4 shows the viscosity of the TiAl4822 alloy.

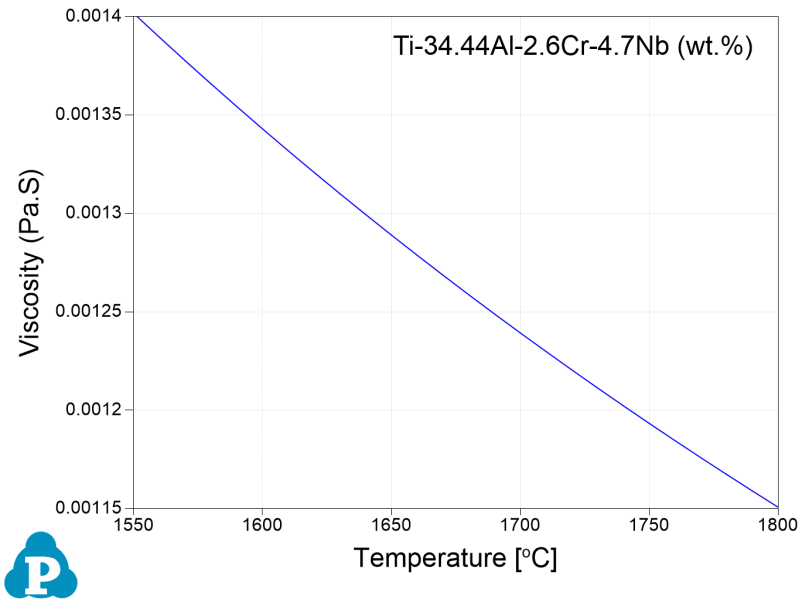

Figure 3.4: Viscosity of the TiAl4822 alloy

4 References

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[2020Ann] Annamalai, A.R.; Srikanth, M.; Varshney, R.; Ashokkumar, M.Y.; Patro, S.K.; Jen, C.-P. Microstructure Evolution and Mechanical Properties of Spark Plasma Sintered Manganese Addition on Ti-48Al-2Cr-2Nb Alloys. Metals, 10 (2020): 1577.

PanTiAl2025: List of Phases

Phases (**208**)

Name	Model	Lattice Size	Constituent
A15	CEF (SLN)	(3)(1)	(Al,Cr,Mo,Nb,Ta,Ti)(Al,Mo,Nb,Sn,Ti)
AL3NBTI4	CEF (ST3)	(3)(1)(4)	(Al)(Nb)(Ti)
A_AlNbTi2	CEF (SLN)	(0.75)(0.25)	(Al,Nb,Ti)(Al,Nb,Ti)
A_TiO	CEF (ST2)	(1)(1)	(Ti)(O)
Al10V	CEF (ST2)	(10)(1)	(Al)(V)
Al11Cr2	CEF (ST2)	(0.846)(0.154)	(Al)(Cr)
Al11Mn4	CEF (ST2)	(11)(4)	(Al)(Mn)
Al11Mn4_HT	CEF (SLN)	(29)(10)	(Al,Mn)(Mn)
Al11Ti5	CEF (ST2)	(17)(8)	(Al)(Ti)
Al12M	CEF (SLN)	(12)(1)	(Al)(Mn,Mo,W)
Al13Cr2	CEF (ST2)	(0.8667) (0.1333)	(Al)(Cr)
Al17Mo4	CEF (ST2)	(17)(4)	(Al)(Mo)
Al22Mo5	CEF (ST2)	(22)(5)	(Al)(Mo)
Al23V4	CEF (ST2)	(23)(4)	(Al)(V)
Al2B51C8	CEF (ST3)	(2)(51)(8)	(Al)(B)(C)
Al2Ti	CEF (SLN)	(2)(1)	(Al,Cr)(Mo,Nb,Ti)
Al2W	CEF (ST2)	(2)(1)	(Al)(W)
Al2Zr3	CEF (ST2)	(2)(3)	(Al)(Zr)
Al3B48C2	CEF (ST3)	(3)(48)(2)	(Al)(B)(C)
Al3BC	CEF (ST3)	(3)(1)(1)	(Al)(B)(C)

Name	Model	Lattice Size	Constituent
Al3BC3	CEF (ST3)	(3)(1)(3)	(Al)(B)(C)
Al3Mo	CEF (ST2)	(3)(1)	(Al)(Mo)
Al3SiB48	CEF (ST3)	(3)(1)(48)	(Al)(Si)(B)
Al3Zr	CEF (ST2)	(3)(1)	(Al)(Zr)
Al3Zr2	CEF (ST2)	(3)(2)	(Al)(Zr)
Al3Zr4	CEF (ST2)	(3)(4)	(Al)(Zr)
Al3Zr5	CEF (SLN)	(3)(5)	(Al)(Ti,Zr)
Al4C3	CEF (SLN)	(4)(3)	(Al,Si)(B,C)
Al4Cr	CEF (ST2)	(0.8)(0.2)	(Al)(Cr)
Al4M	CEF (SLN)	(4)(1)	(Al)(Mo,W)
Al4Mn	CEF (ST2)	(4)(1)	(Al)(Mn)
Al4Mn_L	CEF (ST2)	(461)(107)	(Al)(Mn)
Al4SiC4	CEF (ST3)	(4)(1)(4)	(Al)(Si)(C)
Al4Zr5	CEF (ST2)	(4)(5)	(Al)(Zr)
Al5M	CEF (SLN)	(5)(1)	(Al)(Mo,W)
Al63Mo37	CEF (ST2)	(63)(37)	(Al)(Mo)
Al67M8Ti25	CEF (SLN)	(67)(8)(25)	(Al,Cr,Mn,Ti)(Al,Cr,Mn)(Al,Cr,Mn,Ti)
Al69Ta39	CEF (SLN)	(0.6389) (0.3611)	(Al,Ta,Ti)(Al,Ta)
Al6Mn	CEF (ST2)	(6)(1)	(Al)(Mn)
Al77W23	CEF (ST2)	(77)(23)	(Al)(W)
Al7V	CEF (ST2)	(7)(1)	(Al)(V)
Al7W3	CEF (ST2)	(7)(3)	(Al)(W)
Al8Mn5	CEF (SLN)	(12)(5)(9)	(Al)(Mn)(Al,Mn)
Al8Mo3	CEF (SLN)	(8)(3)	(Al,Ti)(Mo)

Name	Model	Lattice Size	Constituent
Al8SiC7	CEF (ST3)	(8)(1)(7)	(Al)(Si)(C)
Al8V5	CEF (ST2)	(8)(5)	(Al)(V)
AlB12	CEF (ST2)	(1)(12)	(Al)(B)
AlB40C4	CEF (ST3)	(1)(40)(4)	(Al)(B)(C)
AlCr2	CEF (SLN)	(0.333)(0.667)	(Al,Cr)(Al,Cr,Ti)
AlN	CEF (ST2)	(1)(1)	(Al)(N)
AlNbO4	CEF (ST3)	(1)(1)	(Al2O3)(Nb2O5)
AlZr	CEF (ST2)	(1)(1)	(Al)(Zr)
AlZr2	CEF (ST2)	(1)(2)	(Al)(Zr)
Alpha-Mn2B	CEF (ST2)	(0.670691) (0.329309)	(Mn)(B)
Alpha_B	CEF (ST1)	(1)	(B)
Alpha_M5Si3	CEF (SLN)	(5)(3)	(Nb,Ta,W)(Si)
Alpha_MoB	CEF (SLN)	(0.5)(0.5)	(Mo,W)(B,Va)
Alpha_SiZr	CEF (ST2)	(1)(1)	(Zr)(Si)
Alpha_TiMn	CEF (SLN)	(1)(1)	(Cr,Mn)(Ti)
B2	CEF (SLN)	(1)(1)	(Al,Cr,Mn,Mo,Nb,Ti) (Cr,Mn,Mo,Nb,Ti,Va)
B4C	CEF (SLN)	(1)(1)	(B12,B11C)(B2,B2C,BC2,Si2)
BCT_A5	CEF (SLN)	(1)	(Al,Sn)
BETA_VO	CEF (SLN)	(1)(1)	(V)(O,Va)
B_AlNbTi2	CEF (SLN)	(0.5)(0.25) (0.25)	(Al,Nb,Ti)(Al,Nb,Ti)(Al,Nb,Ti)
Bcc	CEF (SLN)	(1)(3)	(Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,V,W,Zr) (B,C,N,O,Va)
Bcc_B2	CEF (SLN)	(0.5)(0.5)(3)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,V,W)

Name	Model	Lattice Size	Constituent
			(Al,Cr,Mn,Mo,Nb,Ta,Ti,V,W)(Va)
Beta_B	CEF (SLN)	(93)(12)	(B)(B,Mn,Si,Zr)
Beta_Cr5Si3	CEF (SLN)	(5)(3)	(Cr)(Cr,Si)
Beta_Si4Zr5	CEF (ST2)	(4)(5)	(Si)(Zr)
Beta_SiZr	CEF (ST2)	(1)(1)	(Si)(Zr)
Beta_TiMn	CEF (ST2)	(0.515)(0.485)	(Mn)(Ti)
Beta_WC	CEF (SLN)	(1)(1)	(Mo,W)(C)
C16	CEF (SLN)	(1)(2)	(Si)(Ta,Zr)
C2V3	CEF (ST2)	(2)(3)	(C)(V)
CBCC_A12	CEF (SLN)	(1)(1)	(Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,V)(C,Va)
CUB_A13	CEF (SLN)	(1)(1)	(Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,V)(C,Va)
Cementite	CEF (SLN)	(3)(1)	(Cr,Mn,Mo)(C)
Corundum	CEF (SLN)	(2)(3)	(Al,Cr,Ti,V)(O)
Cr2B	CEF (SLN)	(0.667)(0.333)	(Cr,Mo)(B)
Cr3Mn5	CEF (ST2)	(3)(5)	(Cr)(Mn)
Cr3Si	CEF (SLN)	(3)(1)(3)	(Cr,Mo,Nb,Si,V)(Cr,Mo,Si,V)(Va)
Cr5B3	CEF (SLN)	(0.625)(0.375)	(Cr,Mo)(B)
CrB	CEF (SLN)	(0.5)(0.5)	(Cr,Mn,Mo,Nb,Ta,Ti,W)(B,Va)
CrB4	CEF (ST2)	(0.2)(0.8)	(Cr)(B)
CrSi	CEF (SLN)	(1)(1)	(Cr,Mn)(Al,Si)
CrSi2	CEF (SLN)	(1)(2)	(Cr,Mo,Nb,Si,Ta,V)(Cr,Si)
Cristobalite	CEF (ST2)	(1)(2)	(Si)(O)
D0_19	CEF (SLN)	(0.75)(0.25) (0.5)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,V,Zr) (Al,Mn,Mo,Nb,Sn,Ta,Ti,Zr)(C,O,N,Va)
D0_22	CEF (SLN)	(0.75)(0.25) (0.5)	(Al,Cr,Mo,Si,Ti)(Al,Cr,Mo,Nb,Ta,Ti,V) (C,Va)

Name	Model	Lattice Size	Constituent
Diamond	CEF (SLN)	(1)	(Al,B,C,Si,Sn,Ti)
Disorder	CEF (SLN)	(1)(1)	(Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,V,W,Zr) (Va)
Fcc	CEF (SLN)	(1)(1)	(Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,V,W,Zr) (B,C,N,O,Va)
GAS	GAS	(1)	(Al,AlO,AlO2,Al2,Al2O,Al2O2,Al2O3, C1O1,C1O2,Mn,O,O2,O3,Sn,Sn2, SnO,SnO2,Si,Si2,Si3,SiO,SiO2, Ti,TiO,TiO2,Zr,Zr2,ZrO,ZrO2)
Gamma	CEF (SLN)	(2)(2)(3)(6)	(Al,Cr,Ti)(Al,Cr,Ti)(Cr)(Al)
Graphite	CEF (SLN)	(1)	(B,C)
H_Sigma_ CrMn	CEF (SLN)	(8)(4)(18)	(Mn)(Cr)(Cr,Mn)
H_Ti2AlC	CEF (SLN)	(2)(1)(1)	(Ti)(Al)(C,Va)
Halite	CEF (SLN)	(1)(1)	(Mn+2,Mn+3,V,V+2,V+3,Va)(O-2,Va)
Hcp	CEF (SLN)	(1)(0.5)	(Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,V,W,Zr) (B,C,N,O,Va)
L10_TiAl	CEF (SLN)	(1)(1)(2)	(Al,Cr,Mn,Mo,Nb,Sn,Ta,Ti,V,W,Zr) (Al,Cr,Mn,Mo,Nb,Sn,Ta,Ti,V,W,Zr) (C,O,N,Va)
L12	CEF (SLN)	(0.75)(0.25)(1)	(Al,Cr,Mn,Mo,Nb,Ti,W,Zr) (Al,Cr,Mn,Mo,Nb,Ti,W,Zr)(Va)
Laves_C14	CEF (SLN)	(2)(1)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,V,Zr) (Al,Cr,Mn,Mo,Nb,Ta,Ti,V,Zr)
Laves_C15	CEF (SLN)	(2)(1)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,V,W,Zr) (Al,Cr,Mn,Mo,Nb,Ta,Ti,V,W,Zr)
Laves_C36	CEF (SLN)	(2)(1)	(Al,Cr,Ti,V,Zr)(Al,Cr,Ti,V,Zr)

Name	Model	Lattice Size	Constituent
Liquid	CEF (SLN)	(1)	(Al,B,C,Cr,Mn,Mo,N,Nb,O,Si,Sn, Ta,Ti,V,W,Zr,Al2O3,Cr2O3,MnO, Mn2/3O,NbO,NbO2,Nb2O5,SiO2, SnO,SnO2,Ta2O5,WO2,WO3,Zr1/2O)
M23C6	CEF (SLN)	(20)(3)(6)	(Cr,Mn,Mo)(Cr,Mn,Mo,W)(C)
M2B	CEF (SLN)	(2)(1)	(Cr,Mn,Mo,Ta,W)(B)
M3B2	CEF (SLN)	(0.6)(0.4)	(Cr,Mo,Nb,Ta,Ti)(B)
M3B4	CEF (SLN)	(3)(4)	(Cr,Mn,Mo,Nb,Ta,Ti)(B)
M3C2	CEF (SLN)	(3)(2)	(Cr,Mo,W)(C)
M3O4	CEF (ST2)	(3)(4)	(Cr)(O)
M3Si	CEF (SLN)	(3)(1)	(Mo,Nb,Ta,Ti,Zr)(Si)
M5Si3	CEF (SLN)	(0.5)(0.125) (0.375)	(Cr,Mo,Nb,Ta,V,W) (Cr,Mo,Nb,Si,Ta,V,W)(Mo,Nb,Si)
M7C3	CEF (SLN)	(7)(3)	(Cr,Mn,Mo,W)(C)
MB	CEF (SLN)	(1)(1)	(Mn,Nb,Ti)(B,C)
MB2	CEF (SLN)	(1)(2)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,Zr,Va)(B,C,Va)
MO2	CEF (SLN)	(1)(2)	(Mo,W,Zr)(O)
MSi2	CEF (SLN)	(1)(2)	(Mo,Nb,W)(Si,Va)
Mn11Si19	CEF (SLN)	(11)(19)	(Mn)(Al,Si)
Mn19Sn6	CEF (ST2)	(19)(6)	(Mn)(Sn)
Mn2Sn	CEF (ST2)	(2)(1)	(Mn)(Sn)
Mn3O4_A	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3O4_B	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3Si	CEF (SLN)	(3)(1)	(Mn)(Al,Si)
Mn3Ti	CEF (ST2)	(3)(1)	(Mn)(Ti)
Mn4Ti	CEF (ST2)	(0.815)(0.185)	(Mn)(Ti)

Name	Model	Lattice Size	Constituent
Mn5C2	CEF (ST2)	(5)(2)	(Mn)(C)
Mn5Si3	CEF (SLN)	(2)(3)(3)(1)	(Mn,Si,Ti,Zr)(Al,Si,Ti)(Mn,Ti,Zr)(C,Va)
Mn6Si	CEF (SLN)	(17)(3)	(Mn)(Al,Si)
Mn9Si2	CEF (ST2)	(33)(7)	(Mn)(Si)
MnB4	CEF (ST2)	(0.2)(0.8)	(Mn)(B)
MnSn2	CEF (ST2)	(1)(2)	(Mn)(Sn)
Mo2B5	CEF (SLN)	(2)(5)	(Mo,W)(B,Va)
Mo3Sn	CEF (ST2)	(3)(1)	(Mo)(Sn)
MoB4	CEF (ST2)	(0.8)(0.2)	(B)(Mo)
MoC_Eta	CEF (SLN)	(1)(1)	(Mo,Ti)(C,Va)
MoSn	CEF (ST2)	(1)(1)	(Mo)(Sn)
MoSn2	CEF (ST2)	(1)(2)	(Mo)(Sn)
Mu	CEF (SLN)	(7)(2)(4)	(Al,Cr,Mn,Mo,Nb)(Mo,Nb,Ti) (Cr,Mo,Nb,Ti)
Nb2B3	CEF (ST2)	(2)(3)	(Nb)(B)
Nb2O5	CEF (ST2)	(2)(5)	(Nb)(O)
Nb3Sn	CEF (SLN)	(3)(1)	(Nb,Sn)(Nb,Sn)
Nb5B6	CEF (SLN)	(5)(6)	(Nb,Ti)(B)
Nb6Sn5	CEF (SLN)	(24)(16)(4)	(Nb)(Sn)(Nb,Sn)
NbO	CEF (ST2)	(1)(1)	(Nb)(O)
NbO2	CEF (ST2)	(1)(2)	(Nb)(O)
NbSn2	CEF (ST2)	(1)(2)	(Nb)(Sn)
P_Ti3AlC	CEF (SLN)	(3)(1)(1)	(Ti)(Al,Ti)(C,Va)
Phi	CEF (SLN)	(0.8837) (1.1163)	(Al,Ta,Ti)(Al,Ta,Ti)

Name	Model	Lattice Size	Constituent
Quartz	CEF (ST2)	(1)(2)	(Si)(O)
Rutile	CEF (SLN)	(1)(2)	(Mn,Sn,Ti,V)(O)
Si2Zr	CEF (ST2)	(2)(1)	(Si)(Zr)
Si2Zr3	CEF (ST2)	(2)(3)	(Si)(Zr)
Si3N4	CEF (ST2)	(3)(4)	(Si)(N)
SiB3	CEF (SLN)	(6)(2)(6)	(B)(Si)(B,Si)
SiB6	CEF (SLN)	(210)(23)(48)	(B)(Si)(B,Si)
SiBn	CEF (SLN)	(61)(1)(8)	(B)(Si)(B,Si)
SiC	CEF (SLN)	(1)(1)	(Si)(B,C)
Sigma	CEF (SLN)	(8)(4)(18)	(Al,Cr,Mn,Ta,W)(Cr,Mo,Nb,Ta,Ti,V,W) (Al,Cr,Mn,Mo,Nb,Ta,Ti,V,W)
Sn2V	CEF (ST2)	(0.333)(0.333) (0.334)	(V)(Sn)(Sn)
Sn2Zr	CEF (ST2)	(2)(1)	(Sn)(Zr)
Sn3Ta2	CEF (ST2)	(3)(2)	(Sn)(Ta)
Sn3Ti2	CEF (ST2)	(0.6)(0.4)	(Sn)(Ti)
Sn3Ti5	CEF (ST2)	(3)(5)	(Sn)(Ti)
Sn3Zr5	CEF (SLN)	(5)(3)(1)	(Zr)(Sn)(Sn,Va)
Sn5Ti6	CEF (ST2)	(5)(6)	(Sn)(Ti)
SnTi2	CEF (ST2)	(1)(2)	(Sn)(Ti)
SnV3	CEF (SLN)	(0.25)(0.75)	(Sn,V)(V)
SnZr4	CEF (SLN)	(3)(1)	(Sn,Zr)(Sn,Zr)
Ta2O5_S	CEF (SLN)	(1)	(Ta,Ta2O5)
Ta2O5_S2	CEF (SLN)	(1)	(Ta,Ta2O5)
Ti2AlN	CEF (ST3)	(2)(1)(0.82)	(Ti)(Al)(N)

Name	Model	Lattice Size	Constituent
Ti2N	CEF (ST2)	(2)(1)	(Ti)(N)
Ti3Al2N2	CEF (ST3)	(3)(2)(2)	(Ti)(Al)(N)
Ti3AlN	CEF (ST3)	(3)(1)(0.56)	(Ti)(Al)(N)
Ti3MC2	CEF (SLN)	(3)(1)(2)	(Ti)(Al,Si)(C,Va)
Ti3N2	CEF (ST2)	(0.71)(0.29)	(Ti)(N)
Ti3O2	CEF (ST2)	(3)(2)	(Ti)(O)
Ti4N3	CEF (ST2)	(0.685)(0.315)	(Ti)(N)
Ti6Si2B	CEF (ST3)	(6)(2)(1)	(Ti)(Si)(B)
Ti7Al5Si12	CEF (SLN)	(7)(1)(16)	(Ti)(Al)(Al,Si)
TiM2	CEF (SLN)	(1)(2)	(Ti)(Al,Si)
TiNb2O7	CEF (ST3)	(1)(1)	(TiO2)(Nb2O5)
TiOx	CEF (SLN)	(1)(1)(1)	(Ti+2,Ti+3,Va)(Ti,Va)(O-2)
TiSi	CEF (SLN)	(0.5)(0.5)	(Ti)(Al,Si)
TiSi2	CEF (SLN)	(1)(2)	(Ti)(Al,Si)
Tridymite	CEF (ST2)	(1)(2)	(Si)(O)
V2B3	CEF (ST2)	(2)(3)	(V)(B)
V3B2	CEF (ST2)	(3)(2)	(V)(B)
V3B4	CEF (ST2)	(3)(4)	(V)(B)
V5B6	CEF (ST2)	(5)(6)	(V)(B)
V6Si5	CEF (ST2)	(0.545455) (0.454545)	(V)(Si)
VB	CEF (ST2)	(1)(1)	(V)(B)
VB2	CEF (ST2)	(1)(2)	(V)(B)
W2B9	CEF (ST2)	(2)(9)	(W)(B)
WO272	CEF (ST2)	(1)(2.72)	(W)(O)

Name	Model	Lattice Size	Constituent
WO290	CEF (ST2)	(1)(2.9)	(W)(O)
WO296	CEF (ST2)	(1)(2.96)	(W)(O)
WO3_A	CEF (ST2)	(1)(3)	(W)(O)
WO3_B	CEF (ST2)	(1)(3)	(W)(O)
Zr2O	CEF (ST2)	(2)(1)	(Zr)(O)
Zr3O	CEF (ST2)	(3)(1)	(Zr)(O)
Zr5Si4	CEF (SLN)	(5)(4)	(Ti,Zr)(Si)
Zr6O	CEF (ST2)	(6)(1)	(Zr)(O)
ZrB	CEF (ST2)	(1)(1)	(Zr)(B)
ZrB12	CEF (ST2)	(1)(12)	(Zr)(B)
ZrO2_Cubic	CEF (SLN)	(1)(2)	(Zr)(O,Va)
ZrO2_Tetra-gonal	CEF (SLN)	(1)(2)	(Zr)(O,Va)