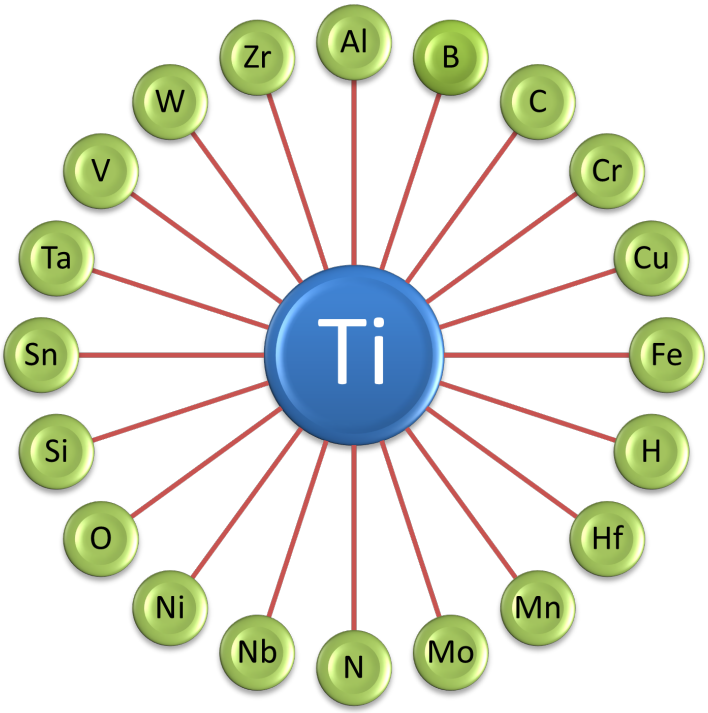
Pandat™ 2024

Database Manual

CompuTherm LLC

PanTitanium

Database for multi-component Titanium-based alloys



PANDAT™ SOFTWARE

Contents

1 Thermodynamic Database

1.1 Components (21)

A total of **21** components are included in the database as listed here:

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

Minor alloying elements: B, C, H, Hf, Mn, N, O and Si

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,	0-35
V	0-11
Mo, Nb, Ta, W, Zr	0-8
Cr,Sn	0-5
Cu, Fe, Ni	0-3
B, C, H, N, O, Hf, Mn, Si	0-0.5

1.3 Phases

A total of **340** phases are included in the current database. The names and thermodynamic models of some phases are given in Table 1.2. Information on all phases is listed in PanTi2024: 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_M3Al	(3)(1)	(Al,Mo,Nb,Ti,V)(Al,Mo,Nb,Ti)
Bcc	(1)(3)	(Al,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Si,Sn,Ta,Ti, V,W,Zr) (B,C,H,N,O,Va)
D0_19	(0.75)(0.25)(0.5)	(Al,Cr,Mn,Mo,Nb,Sn,Ta,Ti,V,Zr) (Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,Zr)(O,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,Cu,Fe,Mn,Mo,Nb,Ni,Si,Sn,Ta,Ti,V,W,Zr) (B,C,H,N,O,Va)
Hcp	(1)(0.5)	(Al,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Si,Sn,Ta,Ti, V,W,Zr) (B,C,H,N,O,Va)
L10_TiAl	(1)(1)(2)	(Al,Cr,Mn,Mo,Nb,Si,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,Fe,Mn,Mo,Nb,Si,Ta,Ti,V,Zr) (Al,Cr,Fe,Mn,Mo,Nb,Ta,Ti,V,W,Zr)
Laves_C15	(2)(1)	(Al,Cr,Mo,Mn,Nb,Si,Ta,Ti,V,W,Zr) (Al,Cr,Mo,Mn,Nb,Si,Ta,Ti,V,Zr)
Laves_C36	(2)(1)	(Al,Cr,Ni,Ti,V,Zr)(Al,Cr,Ni,Ti,V,Zr)
Liquid	(1)	(Al,B,C,Cr,Cu,Fe,H,Hf,Mn,Mo,N,Nb,Ni,O,Si,Sn,Ta, Ti,V,W,Zr,Al2O3,Cr2O3,FeO,HfO2,MoO2,MoO3, NbO, NbO2,Nb2O5,NiO,Si3N4,SiO2,Ta2O5,ZrO2)
Sigma	(8)(4)(18)	(Al,Fe,Mn,Ni,Ta)(Cr,Mo,Nb,Ta,Ti,V) (Al,Cr,Fe,Mn,Mo,Nb,Ni,Ta,Ti,V)

1.4 Assessed Subsystems

A total of **231** subsystems, including 180 binary and 51 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 (180)

Al-B(10)	Al-C(10)	Al-Cr(10)	Al-Cu(10)	Al-Fe(10)	Al-Mn(10)
Al-Mo(10)	Al-Nb(10)	Al-Ni(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-Cu(10)	B-Fe(10)	B-Mn(10)	B-Mo(10)	B-Nb(10)
B-Ni(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-Cu(10)	C-Fe(10)	C-Mn(10)
C-Mo(10)	C-Nb(10)	C-Ni(10)	C-Si(10)	C-Ta(10)	C-Ti(10)
C-V(10)	C-W(10)	C-Zr(10)	Cr-Cu(10)	Cr-Fe(10)	Cr-Mn(10)
Cr-Mo(10)	Cr-N(10)	Cr-Nb(10)	Cr-Ni(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)
Cu-Fe(10)	Cu-Mn(10)	Cu-Mo(10)	Cu-Nb(10)	Cu-Ni(10)	Cu-O(10)
Cu-Si(10)	Cu-Sn(10)	Cu-Ta(10)	Cu-Ti(10)	Cu-V(10)	Cu-W(10)
Cu-Zr(10)	Fe-Mn(10)	Fe-Mo(10)	Fe-Nb(10)	Fe-Ni(10)	Fe-O(10)
Fe-Si(10)	Fe-Sn(10)	Fe-Ta(10)	Fe-Ti(10)	Fe-V(10)	Fe-W(10)
Fe-Zr(10)	H-Ti(10)	H-Zr(10)	Hf-O(10)	Hf-Ta(10)	Hf-Ti(10)
Hf-Nb(10)	Mn-Mo(10)	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-Nb(10)
Mo-Ni(10)	Mo-O(10)	Mo-Si(10)	Mo-Sn(10)	Mo-Ta(10)	Mo-Ti(10)
Mo-V(10)	Mo-Zr(10)	Nb-Ni(10)	Nb-O(10)	Nb-Si(10)	Nb-Sn(10)
Nb-Ti(10)	Nb-V(10)	Nb-W(10)	Nb-Zr(10)	Ni-O(10)	Ni-Si(10)
Ni-Sn(10)	Ni-Ta(10)	Ni-Ti(10)	Ni-V(10)	Ni-W(10)	Ni-Zr(10)

O-Si(10)	O-Sn(10)	O-Ta(10)	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-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)
Al-H(8)	Al-N(8)	H-Nb(8)	H-V(8)	Mn-N(8)	Mo-N(8)
N-Nb(8)	N-Ni(8)	N-Si(8)	N-Sn(8)	N-Ta(8)	N-Ti(8)
N-V(8)	N-Zr(8)	O-Ti(8)	O-V(8)	Cr-H(6)	Cu-H(6)
Cu-N(6)	Fe-H(6)	Fe-N(6)	H-Mn(6)	H-Mo(6)	H-Ni(6)
H-Si(6)	H-Sn(6)	H-Ta(6)	H-W(6)	B-Hf(0)	C-Hf(0)

Ternary Systems (51)

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

1.5 Database Validation

Since this database has been designed for use with conventional α-β types of titanium alloys, it has been focused at the Ti-rich corner. This database has been tested by a large number of α-β type of titanium alloys, such as Ti64, Ti6242 and Ti6246. Table 1.3 lists the alloys and references used for validating the current database. The suggested composition ranges given in Table 1.1 are based on the compositions of these testing alloys. Users need to be careful while using the database beyond the suggested ranges.

This database can be used to calculate phase equilibria for multi-component alloys, such as equilibrium between α and β. It can be used to predict phase transformation temperatures, such as β-transus. The fraction of each phase as a function of temperature, partitioning of components in different phases can also be calculated. In addition to equilibrium calculations, Scheil simulations can also be carried out using this database. Some calculated examples are given below.

Table 1.3: Experimental Data Used for Testing PanTi Database

Alloy	Experimental Information	References
Ti64	β transus, β approach curve, partitioning of Al and V in α and β.	[1966Cas,1979Las, 1986Kah,1986Ro, 1991Lee, 2003Fur, 2003Sem,2003Ven]
Ti-144A	β transus, β approach curve, and/or partition coefficient	[2003Ven]
Ti-155A	β transus, β approach curve, and/or partition coefficient	[2003Ven]
Ti-6246	β transus	[2003Fur]
Ti-6242	β transus	[2003Fur]
IMI 834	β transus	[2003Fur]
Ti-17	β transus	[2003Fur]
Ti-10-2-3	β transus	[2003Fur]
Ti-6-6-2	β transus	[2003Fur]
Ti-62222	β transus	[2003Fur]
Ti-6Al-2Nb-1Ta-0.8Mo	β transus	[1984Lin]

Alloy	Experimental Information	References
Corona X	β approach curve	[2003Boy]
Ti-4.5Al-5Mo-1.5Cr (Corona 5)	β transus	[1984Yod]
Ti-10-2-3	β transus, β approach curve	[1980Due]
IMI 550	β transus, β approach curve, partitioning of Al, Mo, Sn and Si in α and β.	[2001Kha]
α, α+β, and β alloys listed in the handbook	β transus	[1994Boy]

Beta transus, the temperature at which α starts to form from β, is an important reference parameter in the selection of processing conditions, such as heat treatment process, for the conventional α-β type of titanium alloys. This temperature has been calculated for a large number of Ti64 and other titanium alloys using the current database. Figure 1.1 shows a comparison between the predicted and observed beta transus temperatures for more than 150 Ti64 heats, reasonable agreement is obtained. The accuracy of the prediction depends on the reliability of the database and the accuracy of the input chemistry of the alloy. The calculated beta transus temperature is found to be very sensitive to the amount of the interstitial elements, such as C, H, N, and O. It is seen from Figure 1.1 that the predicted beta transus temperatures are in agreement with the observed ones. Figure 1.2 shows a similar comparison for other titanium alloys, including Ti662, Ti6242, Ti6246, Ti17 and so on, and reasonable agreement is obtained.

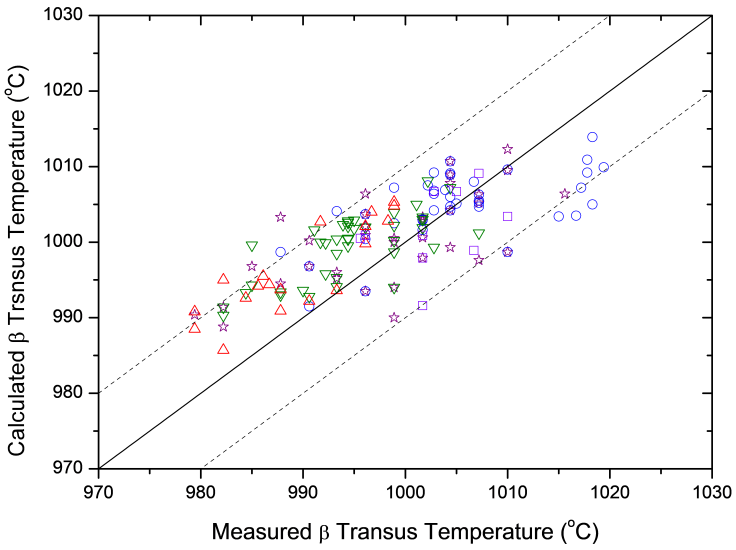


Figure 1.1: Comparison between the predicted and observed beta transus for more than 150 Ti64 heats. The calculated transformation temperatures correspond to 0% of α phase formed and the experimental data are from [1966Cas, 2003Sem, 2003Fur]

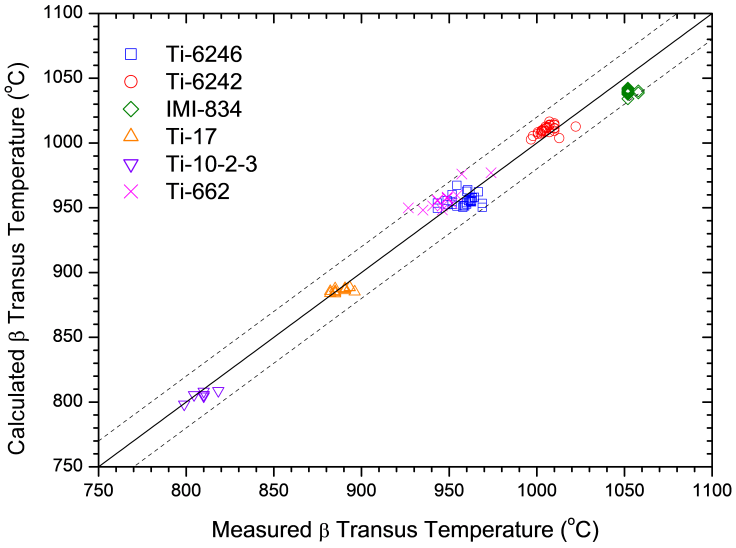


Figure 1.2: Comparison between the predicted and observed beta transus for other titanium alloys. The calculated transformation temperatures correspond to 0% of α phase formed

The relative amounts of α and β phases are critical in the determination of alloy properties for an α-β alloy. Beta approach curve, the volume fraction of beta phase as a function of temperature, is therefore important in the selection of final heat treatment temperature. Beta approach curves for two Ti64 heats are calculated as plotted in Figure 1.3 and Figure 1.4. The experimental data [2003Sem, 1966Cas] are also plotted on the diagrams for comparison; very good agreements are obtained.

It should point out that the calculated phase fractions are mole fractions, while the measured values are volume fractions. However, since the molar volume of the α phase is very close to that of the β phase, the error induced due to the direct comparison between them is small. This can be seen in Figure 1.3 in which both the mole factions and the volume fractions of β phase are plotted.

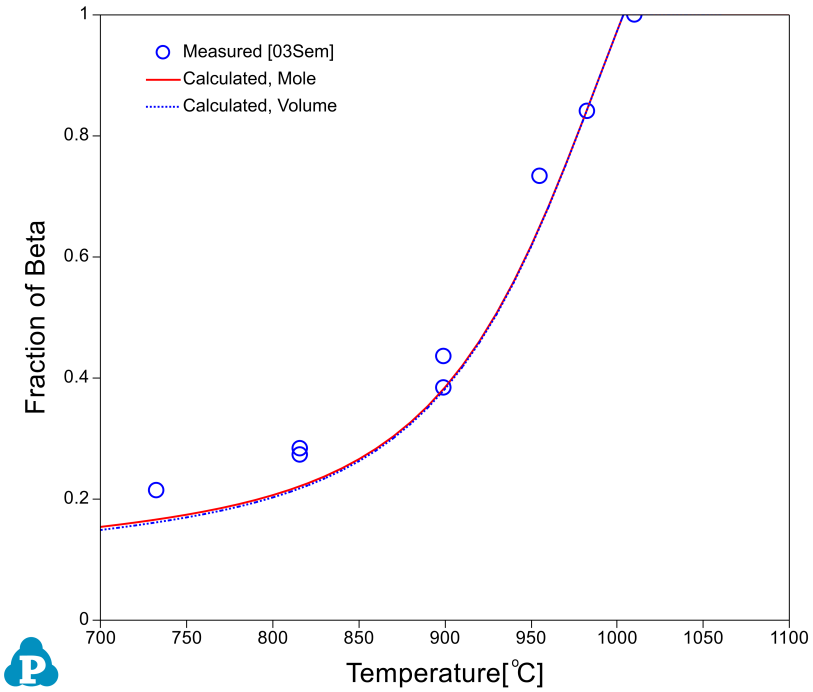


Figure 1.3: Beta approach curve for a Ti64 alloy with experimental data from [2003Sem]

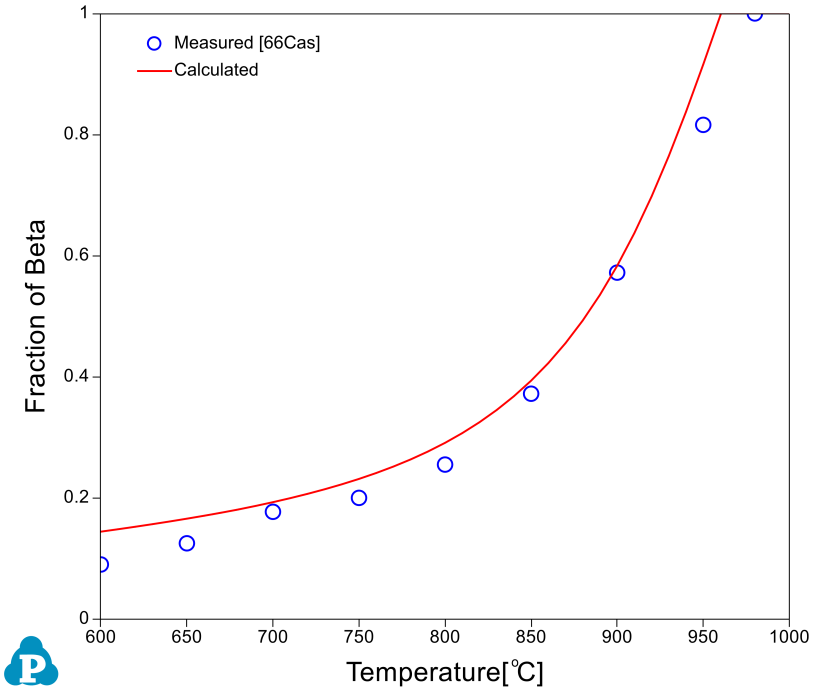


Figure 1.4: Beta approach curve for a Ti64 alloy with experimental data from [1966Cas]

In addition to Ti64, beta approach curves are also calculated for other titanium alloys. Figure 1.5 shows the beta approach curve for one Ti6242 alloy, and the experimental data are from Semiatin [2005Sem].

Equilibrium phase compositions are useful in understanding the partitioning of elements in different phases. These are calculated and compared with the experimental measurements for Ti64 and Ti6242 alloys. Figure 1.6 shows the equilibrium compositions of Al and V in α and β for one Ti64 alloy. In general, the calculated equilibrium compositions agree with the experimental data very well. The calculated Al concentrations in the β phase are higher than the measurements at low temperatures. This is due to the fact that the β grains were too small to allow an accurate analysis [1979Las]. Figure 1.7 shows the equilibrium compositions of Al and Mo in α and β for the Ti6242 alloy.

Figure 1.8 ~ Figure 1.10 show the calculated fractions of α for IMI550, Corona-X and Ti-10-2-3 alloys, respectively. The calculated results agree with experimental data very well.

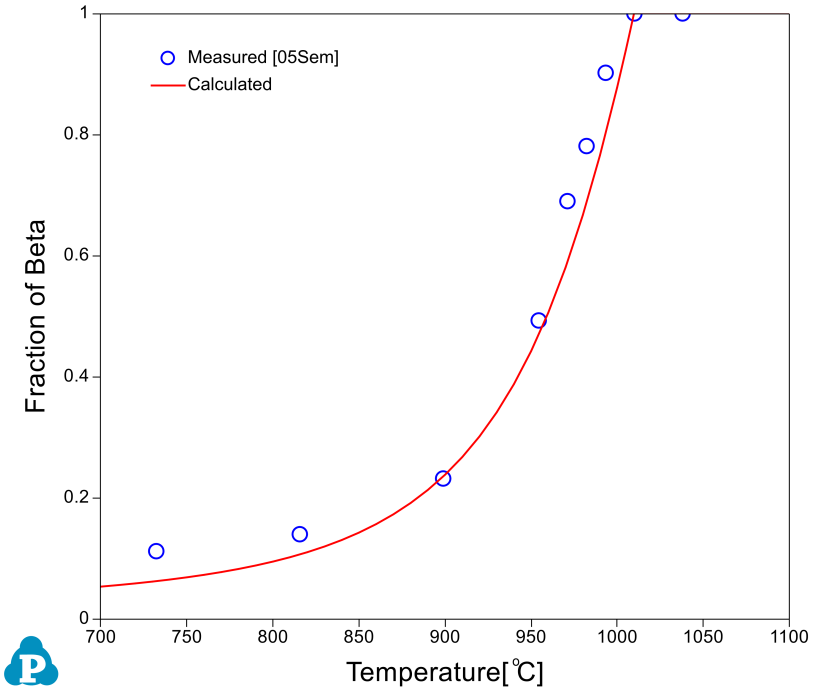


Figure 1.5: Beta approach curve for a Ti-6242 alloy with experimental data from [2005Sem]

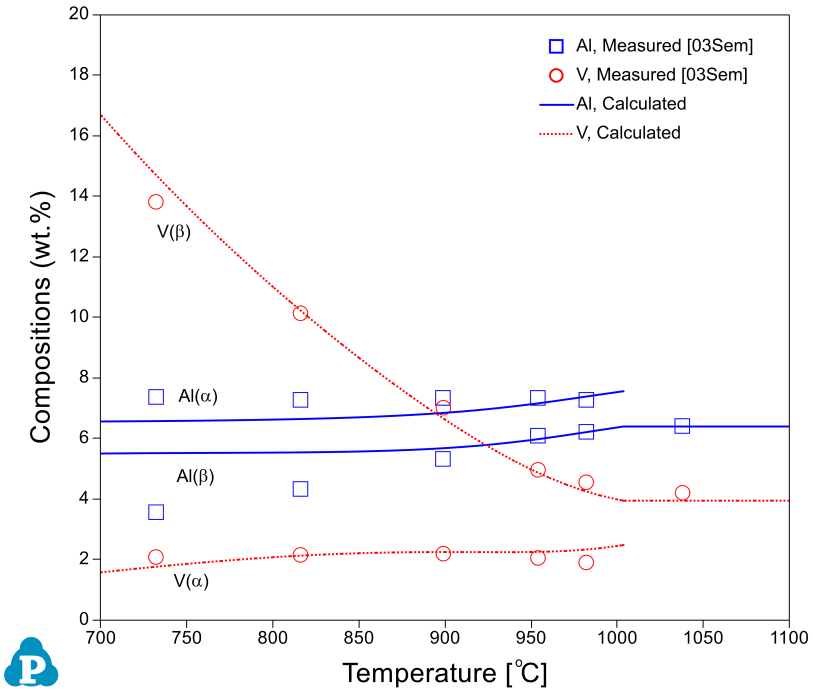


Figure 1.6: Equilibrium compositions of Al and V in the α and β phases for a Ti64 alloy with the experimental data from [2003Sem]

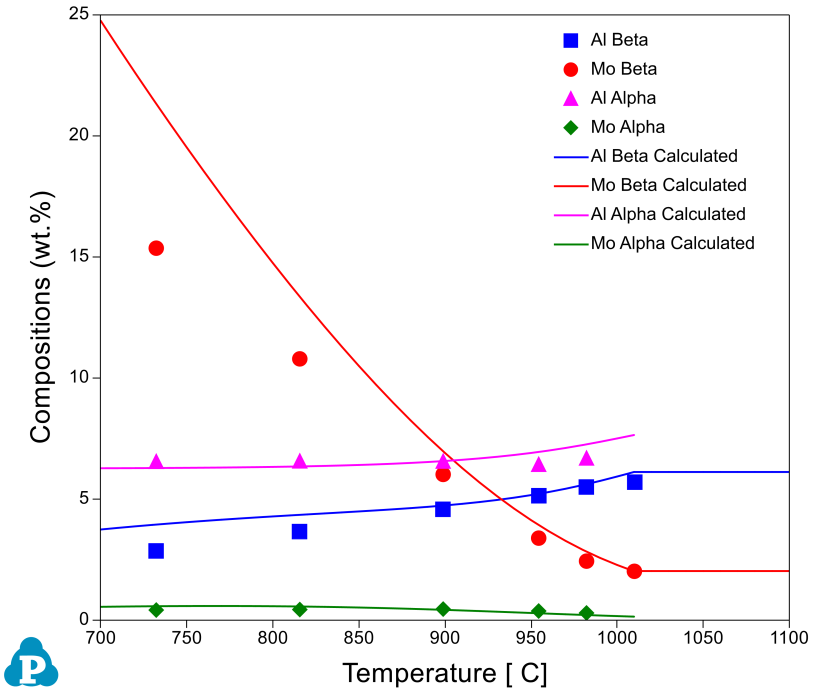


Figure 1.7: Equilibrium compositions of Al and Mo in the alpha and beta phases for a Ti6242 alloy with the experimental data from [2005Sem]

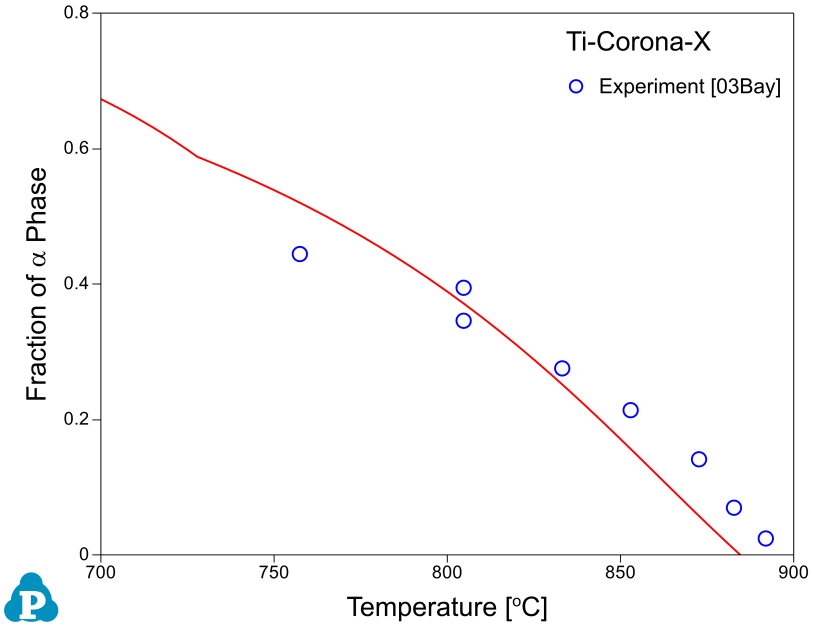


Figure 1.8: Alpha fraction curve for an IMI550 alloy with experimental data [2001Kha]

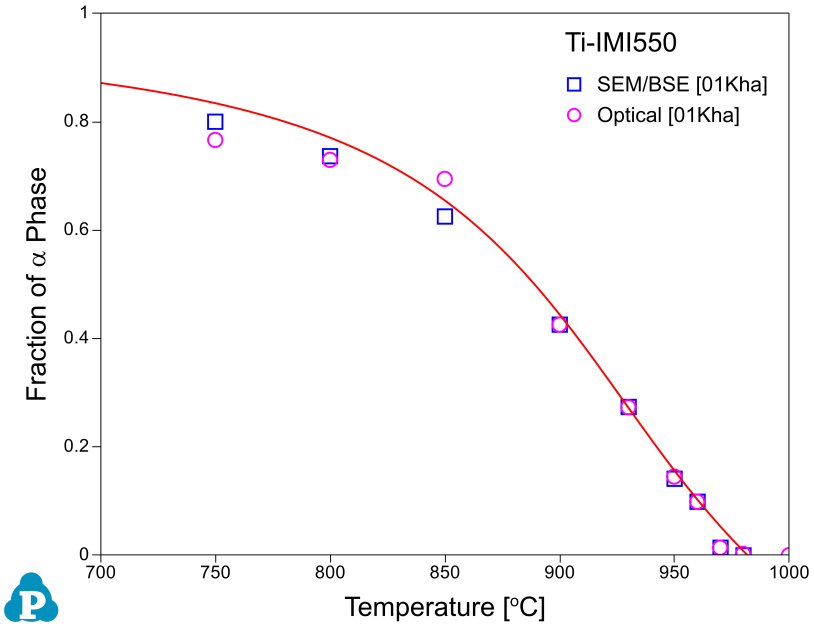


Figure 1.9: Alpha fraction curve for a Corona-X alloy with experimental data [2001Kha]

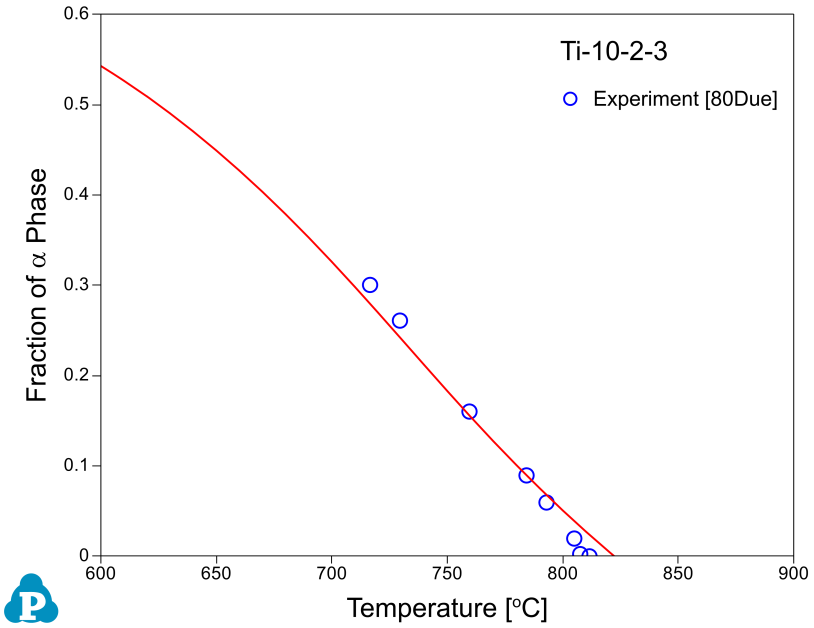


Figure 1.10: Alpha fraction curve for a Ti-10-2-3 alloy with experimental data [1980Due]

2 Mobility Database

PanTi2024_MB is an atomic mobility database for Ti-based alloys, which is compatible with the `PanTi2024_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	Cu	Fe	Hf	Mn	Mo	Nb	Ni	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 and Fcc phases.

Fcc Phase

Al-Si	Al-W	Cr-Ni

Bcc phase

Al-Ti	Cr-Ti	Mo-Nb	Mo-Ta	Mo-Ti	Mo-W	Mo-Zr	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 `PanTi2024_MB` database.

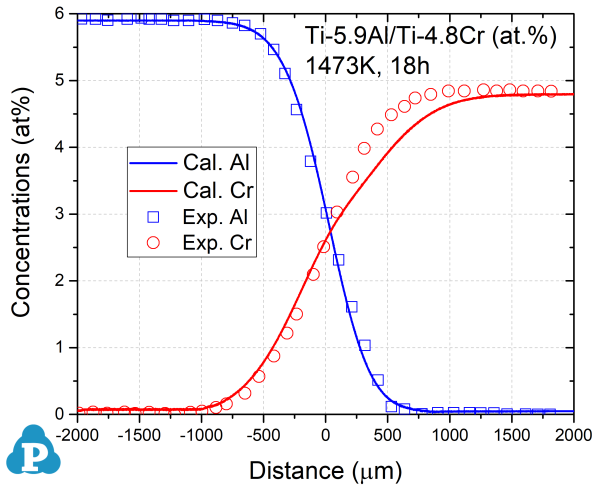


Figure 2.1: Concentration profiles of Ti-5.9Al/Ti-4.8Cr (at.%) at 1473K for 18h [2011Li]

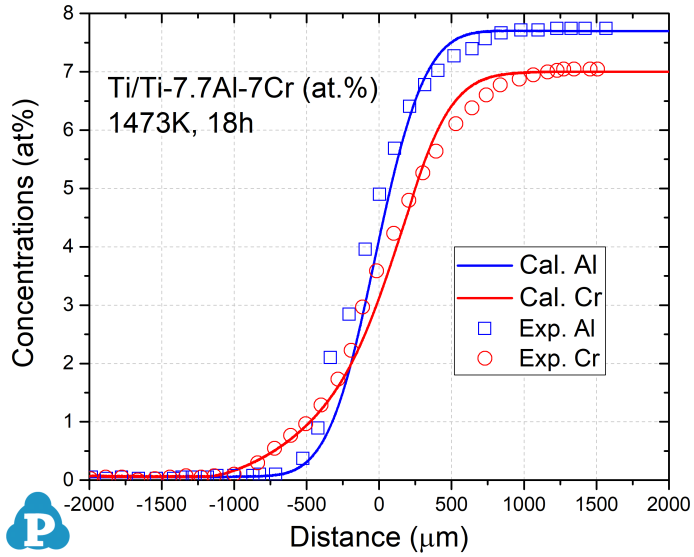


Figure 2.2: Concentration profiles of Ti/Ti-7.7Al-7Cr (at.%) at 1473K for 18h[2011Li]

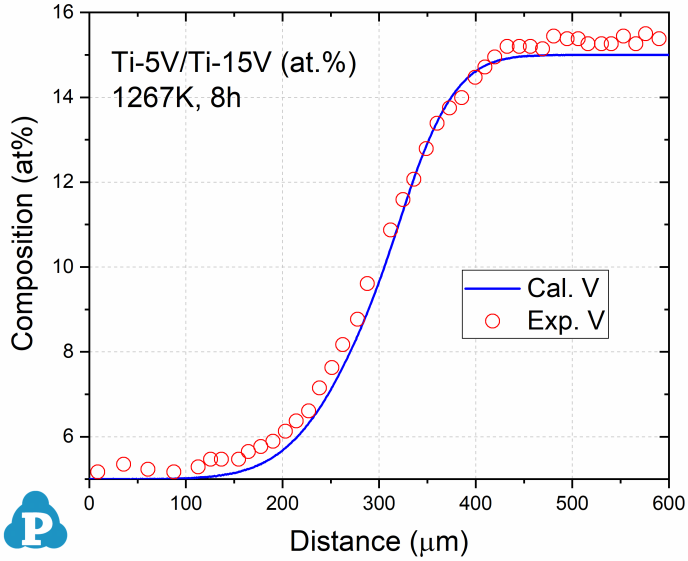


Figure 2.3: Concentration profile of Ti-5V/Ti-15V (at.%) annealed at 1267K for 8h [2009Liu]

3 Thermophysical Property Database

The thermophysical property database **PanTi2024_TP** is compatible with the `PanTi2024_TH` thermodynamic database and suitable for the simulation of thermophysical properties of Ti-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 **340** phases assessed in the `PanTi2024_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 Ti-based alloys are shown below to validate the current database.

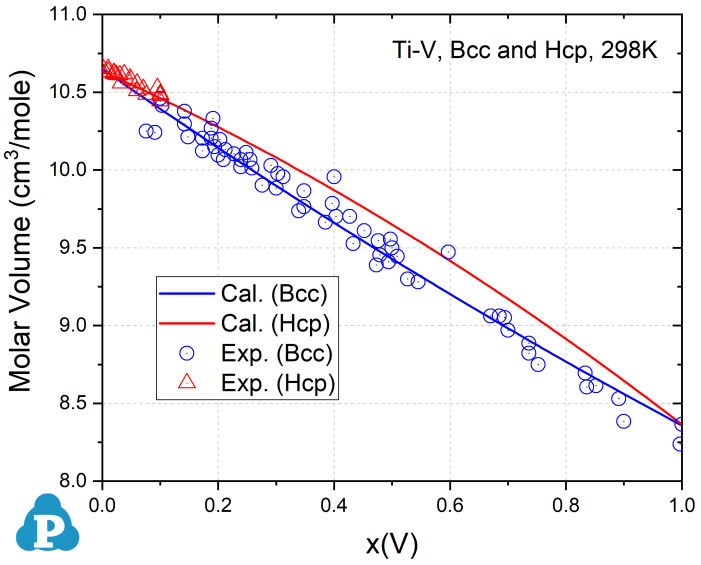


Figure 3.1: Molar volume of Ti-V Bcc and Hcp binary alloys at 298K [2016Yan]

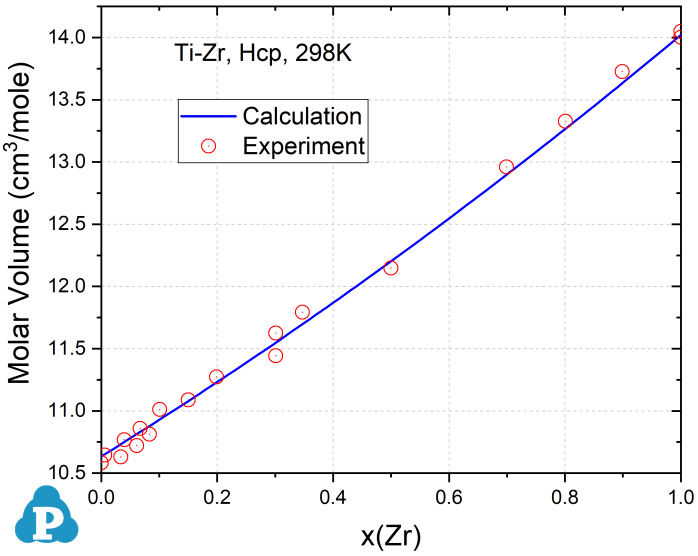


Figure 3.2: Molar volume of Ti-Zr Hcp binary alloys at 298K [2016Yan]

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 Ti-6Al-4V(wt.%) alloy.

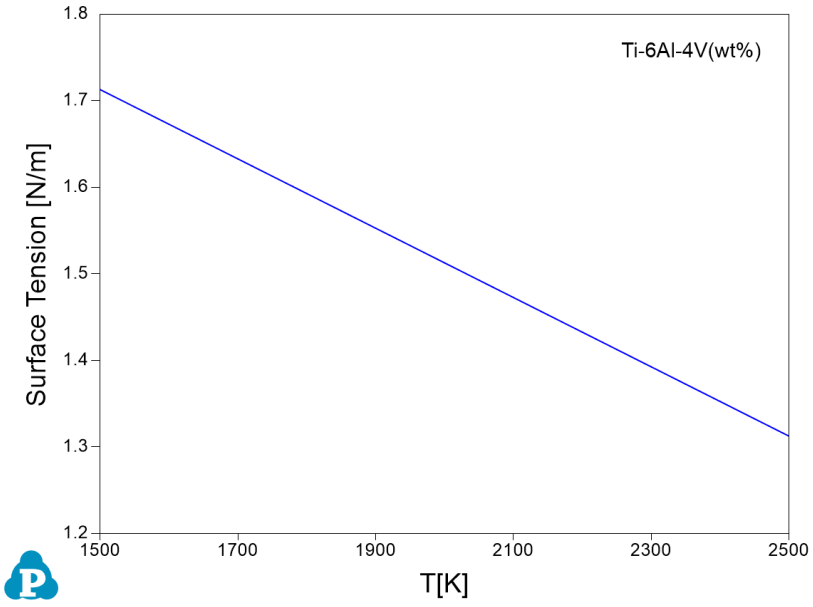


Figure 3.3: Surface tension of the Ti-6Al-4V(wt.%) alloy

3.3 Viscosity

The viscosity of the liquid phase is added into the property database. Figure 3.4 shows the viscosity of the Ti-6Al-4V(wt.%) alloy.

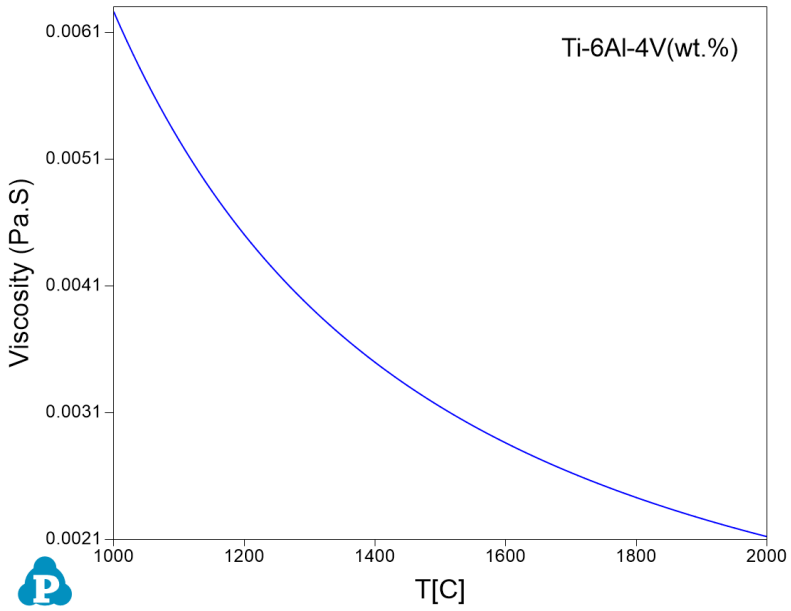


Figure 3.4: Viscosity of the Ti-6Al-4V(wt.%) alloy.

4 References

[1966Cas] R. Castro and L. Seraphin, Mem. Sci. Rev. Met. 63 (1966): 1025-1058.

[1979Las] A.L. Lasalmonie and M.Loubradou, J. Mat. Sci. 14 (1979): 2589-2595.

[1980Due] T.W. Duerig, G.T. Terlinde and J.C. Williams, Met. Trans. A 11A (1980): 1987-1998.

[1984Lin] F. S. Lin, E. A. Starke, Jr., S. B. Chakrabortty and A. Gysler, Met. Trans. 15A (1984): 1229-1246.

[1984Yod] G.R. Yoder, F.H. Froes and D. Eylon, Met. Trans. 15A (1984): 183-197.

[1986Kah] A.I. Kahveci and G.E. Welsch, Scripta Met. 20 (1986): 1287-1290.

[1986Ro] Y. Ro, H. Onodera, and K. Ohno, Trans. Iron Steel Inst. Japan 26(4) (1986): 322-327.

[1991Lee] Y.T. Lee, M. Peters and G. Welsch, Met. Trans. 22A (1991): 709-714.

[1994Boy] R. Boyer, G. Welsch and E. W. Collings, Materials Properties Handbook: Titanium Alloys, ASM International, Materials Park, OH, 1994.

[2001Kha] K.K. Kharia and H.J. Rack, Met. Trans. 32A (2001): 671-679.

[2003Boy] R. Boyer, Boeing, private communication, 2003.

[2003Fur] D. Furrer, LADISH, private communication, 2003.

[2003Sem] S.L. Semiatin, S.L. Knisley, P.N. Fagin, F. Zhang and D.R. Barker, Met. Trans. 34A (2003): 2377-2386.

[2003Ven] V. Venkatesh, TIMET, private communication, 2003.

[2005Sem] S.L. Semiatin, AFRL, private communication, 2005.

[2009Liu] Y. Liu, et al., Assessment of the diffusional mobilities in bcc Ti-V alloys. Journal of Alloys and Compounds, 470 (2009): 176-182.

[2011Li] W. Li, et al., Assessment of diffusion mobility for the bcc phase of the Ti-Al-Cr system. Calphad, 35 (2011): 384-390.

[2016Yan] J.-Y. Yan and G.B. Olson, Molar volumes of bcc, hcp, and orthorhombic Ti-base solid solutions at room temperature. Calphad, 52 (2016):152-158.

PanTi2024: List of Phases

Phases (**340**)

Name	Model	Lattice Size	Constituent
A15_M3Al	CEF (SLN)	(3)(1)	(Al,Mo,Nb,Ti,V)(Al,Mo,Nb,Ti)
AL3NBTI4	CEF (ST3)	(3)(1)(4)	(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 (SLN)	(11)(4)	(Al)(Fe,Mn)
Al11Mn4_HT	CEF (SLN)	(29)(10)	(Al,Mn)(Mn)
Al12Mn	CEF (SLN)	(12)(1)	(Al)(Fe,Mn)
Al12Mo	CEF (ST2)	(12)(1)	(Al)(Mo)
Al12W	CEF (ST2)	(12)(1)	(Al)(W)
Al13Cr2	CEF (ST2)	(0.8667) (0.1333)	(Al)(Cr)
Al13Fe4	CEF (SLN)	(0.6275) (0.235) (0.1375)	(Al)(Fe)(Al,Va)
Al17Mo4	CEF (ST2)	(17)(4)	(Al)(Mo)
Al22Mo5	CEF (ST2)	(22)(5)	(Al)(Mo)
Al23V4	CEF (ST2)	(23)(4)	(Al)(V)
Al2Fe	CEF (ST2)	(2)(1)	(Al)(Fe)
Al2W	CEF (ST2)	(2)(1)	(Al)(W)
Al2Zr3	CEF (ST2)	(2)(3)	(Al)(Zr)

Name	Model	Lattice Size	Constituent
Al3Mo	CEF (ST2)	(3)(1)	(Al)(Mo)
Al3Ni	CEF (ST2)	(0.75)(0.25)	(Al)(Ni)
Al3Ni2	CEF (SLN)	(3)(2)(1)	(Al)(Al,Ni)(Ni,Va)
Al3Ni5	CEF (ST2)	(0.375)(0.625)	(Al)(Ni)
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 (ST2)	(4)(3)	(Al)(C)
Al4Cr	CEF (ST2)	(0.8)(0.2)	(Al)(Cr)
Al4Mn	CEF (SLN)	(4)(1)	(Al)(Fe,Mn)
Al4Mn_L	CEF (ST2)	(461)(107)	(Al)(Mn)
Al4Mo	CEF (ST2)	(4)(1)	(Al)(Mo)
Al4W	CEF (ST2)	(4)(1)	(Al)(W)
Al4Zr5	CEF (ST2)	(4)(5)	(Al)(Zr)
Al5Fe2	CEF (ST2)	(5)(2)	(Al)(Fe)
Al5Fe4	CEF (SLN)	(1)	(Al,Fe)
Al5Mo	CEF (ST2)	(5)(1)	(Al)(Mo)
Al5W	CEF (ST2)	(5)(1)	(Al)(W)
Al63Mo37	CEF (ST2)	(63)(37)	(Al)(Mo)
Al69Ta39	CEF (SLN)	(0.6389) (0.3611)	(Al,Ta,Ti)(Al,Ta)
Al6Mn	CEF (SLN)	(6)(1)	(Al)(Fe,Mn)
Al77W23	CEF (ST2)	(77)(23)	(Al)(W)
Al7V	CEF (ST2)	(7)(1)	(Al)(V)

Name	Model	Lattice Size	Constituent
Al7W3	CEF (ST2)	(7)(3)	(Al)(W)
Al8Mn5	CEF (SLN)	(12)(5)(9)	(Al,Si)(Mn)(Al,Fe,Mn)
Al8Mo3	CEF (ST2)	(8)(3)	(Al)(Mo)
Al8V5	CEF (SLN)	(8)(5)	(Al)(Fe,Mo,V)
AlB12	CEF (ST2)	(1)(12)	(Al)(B)
AlCr2	CEF (SLN)	(0.333)(0.667)	(Al,Cr)(Al,Cr,Ti)
AlCu_Delta	CEF (ST2)	(0.4)(0.6)	(Al)(Cu)
AlCu_Eps	CEF (SLN)	(0.5)(0.5)	(Al,Cu)(Cu)
AlCu_Eta	CEF (SLN)	(0.5)(0.5)	(Al,Cu)(Cu)
AlCu_Gamma	CEF (SLN)	(4)(1)(8)	(Al)(Al,Cu)(Cu)
AlCu_Gamma_H	CEF (SLN)	(4)(1)(8)	(Al)(Al,Cu)(Cu)
AlCu_Theta	CEF (SLN)	(0.667)(0.333)	(Al)(Al,Cu)
AlCu_Zeta	CEF (ST2)	(0.45)(0.55)	(Al)(Cu)
AlH3	CEF (ST2)	(1)(3)	(Al)(H)
AlMo	CEF (SLN)	(1)(1)	(Al,Mo)(Al,Mo)
AlN	CEF (ST2)	(1)(1)	(Al)(N)
AlZr	CEF (ST2)	(1)(1)	(Al)(Zr)
AlZr2	CEF (ST2)	(1)(2)	(Al)(Zr)
AlZr3	CEF (ST2)	(1)(3)	(Al)(Zr)
Alpha-Mn2B	CEF (ST2)	(0.670691) (0.329309)	(Mn)(B)
Alpha_AlNbTi2	CEF (SLN)	(0.75)(0.25)	(Al,Nb,Ti)(Al,Nb,Ti)
Alpha_B	CEF (ST1)	(1)	(B)
Alpha_MoB	CEF (SLN)	(0.5)(0.5)	(Mo,W)(B,Va)

Name	Model	Lattice Size	Constituent
Alpha_SiZr	CEF (ST2)	(1)(1)	(Zr)(Si)
Alpha_Ta5Si3	CEF (ST2)	(5)(3)	(Ta)(Si)
Alpha_TiMn	CEF (ST2)	(1)(1)	(Mn)(Ti)
Alpha_WB	CEF (SLN)	(1)(1)	(W)(B,Va)
B2	CEF (SLN)	(1)(1)	(Al,Cu,Ni,Ti)(Ni,Ti,Va)
B4C	CEF (SLN)	(1)(1)	(B12,B11C)(B2,B2C,BC2)
BCT_A5	CEF (SLN)	(1)	(Al,Sn,Ti)
BETA_VO	CEF (SLN)	(1)(1)	(V)(O,Va)
Bcc	CEF (SLN)	(1)(3)	(Al,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Si, Sn,Ta,Ti,V,W,Zr)(B,C,H,N,O,Va)
Bcc_B2	CEF (SLN)	(0.5)(0.5)(3)	(Al,Cr,Fe,Mo,Nb,Si,Ti,V) (Al,Cr,Fe,Mo,Nb,Si,Ti,V)(Va)
Beta-Mn2B	CEF (ST2)	(0.666667) (0.333333)	(Mn)(B)
Beta2_Ni3Si	CEF (ST2)	(3)(1)	(Ni)(Si)
Beta3_Ni3Si	CEF (ST2)	(3)(1)	(Ni)(Si)
Beta_ALNBTI2	CEF (SLN)	(0.5)(0.25) (0.25)	(Al,Nb,Ti)(Al,Nb,Ti)(Al,Nb,Ti)
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_Ta5Si3	CEF (ST2)	(5)(3)	(Ta)(Si)
Beta_TiMn	CEF (ST2)	(0.515)(0.485)	(Mn)(Ti)
Beta_WB	CEF (SLN)	(1)(1)	(W)(B,Va)
C2V3	CEF (ST2)	(2)(3)	(C)(V)

Name	Model	Lattice Size	Constituent
CBCC_A12	CEF (SLN)	(1)(1)	(Al,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Si,Sn, Ta,Ti,V)(C,Va)
CUB_A13	CEF (SLN)	(1)(1)	(Al,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Si,Sn, Ta,Ti,V)(C,Va)
Corundum	CEF (SLN)	(2)(3)	(Al,Cr,Fe,Ti,V)(O)
Cr2B	CEF (SLN)	(0.667)(0.333)	(Cr,Mo)(B)
Cr2O3	CEF (ST2)	(2)(3)	(Cr)(O)
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 (ST2)	(1)(1)	(Cr)(Si)
CrSi2	CEF (SLN)	(1)(2)	(Cr,Mo,Nb,Si,Ta,V)(Cr,Si)
Cristobalite	CEF (ST2)	(1)(2)	(Si)(O)
Cu10Sn3	CEF (SLN)	(1)	(Cu,Sn)
Cu10Zr7	CEF (ST2)	(10)(7)	(Cu)(Zr)
Cu12Nb3Ti5	CEF (ST3)	(0.6)(0.15) (0.25)	(Cu)(Nb)(Ti)
Cu15Si4	CEF (ST2)	(0.789474) (0.210526)	(Cu)(Si)
Cu19Si6	CEF (ST2)	(0.76)(0.24)	(Cu)(Si)
Cu2NbTi2	CEF (ST3)	(0.4)(0.2)(0.4)	(Cu)(Nb)(Ti)
Cu2O	CEF (ST2)	(2)(1)	(Cu)(O)
Cu2Ti	CEF (ST2)	(0.666667) (0.333333)	(Cu)(Ti)

Name	Model	Lattice Size	Constituent
Cu33Si7	CEF (ST2)	(0.825)(0.175)	(Cu)(Si)
Cu3Sn	CEF (SLN)	(3)(1)	(Cu,Sn)(Cu,Sn)
Cu3Ti2	CEF (ST2)	(0.6)(0.4)	(Cu)(Ti)
Cu41Sn11	CEF (SLN)	(41)(11)	(Cu,Sn)(Cu,Sn)
Cu4Ti	CEF (SLN)	(0.8)(0.2)	(Cu,Ti)(Cu,Nb,Ti)
Cu4Ti3	CEF (ST2)	(0.57143) (0.42857)	(Cu)(Ti)
Cu51Zr14	CEF (ST2)	(51)(14)	(Cu)(Zr)
Cu5Zr	CEF (ST2)	(5)(1)	(Cu)(Zr)
Cu6Sn5H	CEF (SLN)	(1)(1)(1)	(Cu)(Cu,Sn)(Sn)
Cu6Sn5L	CEF (SLN)	(1)(1)(1)	(Cu)(Cu,Sn)(Sn)
Cu8Zr3	CEF (ST2)	(8)(3)	(Cu)(Zr)
CuNi2Ti	CEF (ST3)	(0.25)(0.5) (0.25)	(Cu)(Ni)(Ti)
CuNiTi	CEF (SLN)	(0.666667) (0.333333)	(Cu,Ni)(Ti)
CuO	CEF (ST2)	(1)(1)	(Cu)(O)
CuTi	CEF (SLN)	(0.5)(0.5)	(Cu,Ti)(Cu,Nb,Ti)
CuZr	CEF (ST2)	(1)(1)	(Cu)(Zr)
CuZr2	CEF (SLN)	(1)(2)	(Cu,Ni)(Al,Nb,Ti,Zr)
D0_19	CEF (SLN)	(0.75)(0.25) (0.5)	(Al,Cr,Mn,Mo,Nb,Sn,Ta,Ti,V,Zr) (Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,Zr) (O,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)
Delta_Ni2Si	CEF (ST2)	(2)(1)	(Ni)(Si)

Name	Model	Lattice Size	Constituent
Diamond_A4	CEF (SLN)	(1)	(Al,C,Si,Ti)
Epsilon_Ni3Si2	CEF (ST2)	(3)(2)	(Ni)(Si)
Fcc	CEF (SLN)	(1)(1)	(Al,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Si,Sn, Ta,Ti,V,W,Zr)(B,C,H,N,O,Va)
Fe23Zr6	CEF (ST2)	(0.793)(0.207)	(Fe)(Zr)
Fe2Si	CEF (ST2)	(2)(1)	(Fe)(Si)
Fe2Ta_C14	CEF (SLN)	(2)(1)	(Fe,Ta)(Fe,Ta)
Fe3Si7	CEF (ST2)	(0.3)(0.7)	(Fe)(Si)
Fe3Sn2	CEF (ST2)	(3)(2)	(Fe)(Sn)
Fe4N	CEF (SLN)	(4)(1)	(Cr,Fe,Mn,Ni)(C,N,Va)
Fe5Si3	CEF (ST2)	(5)(3)	(Fe)(Si)
Fe5Sn3	CEF (ST2)	(5)(3)	(Fe)(Sn)
FeB	CEF (ST2)	(1)(1)	(Fe)(B)
FeNi3_L12	CEF (SLN)	(0.25)(0.25) (0.25)(0.25)(1)	(Fe,Ni)(Fe,Ni)(Fe,Ni)(Fe,Ni)(Va)
FeSi	CEF (ST2)	(1)(1)	(Fe)(Si)
FeSi2	CEF (ST2)	(1)(2)	(Fe)(Si)
FeSn	CEF (ST2)	(1)(1)	(Fe)(Sn)
FeSn2	CEF (ST2)	(1)(2)	(Fe)(Sn)
FeZr2	CEF (SLN)	(1)(2)	(Fe,Zr)(Fe,Zr)
FeZr3	CEF (SLN)	(1)(3)	(Fe,Zr)(Fe,Zr)
GAS	GAS	(1)	(Al,AlO,AlO2,Al2,Al2O,Al2O2, Al2O3,C1O1,C1O2,Fe,FeO, FeO2,Fe2,Hf,HfO,HfO2,Mn, Mo,MoO2,O,O2,O3,Sn,Sn2, SnO,SnO2,Si,Si2,Si3,SiO,SiO2,

Name	Model	Lattice Size	Constituent
			Ti,TiO,TiO2,Zr,Zr2,ZrO,ZrO2)
Gamma	CEF (SLN)	(2)(2)(3)(6)	(Al,Cr,Ti)(Al,Cr,Ti)(Cr)(Al)
Gamma_CuSn	CEF (SLN)	(1)	(Cu,Sn)
Gamma_Ni5Si2	CEF (ST2)	(5)(2)	(Ni)(Si)
Graphite	CEF (ST1)	(1)	(C)
H_Sigma_CrMn	CEF (SLN)	(8)(4)(18)	(Mn)(Cr)(Cr,Mn)
Halite	CEF (SLN)	(1)(1)	(Cr,Fe,Ni,V)(O)
Hcp	CEF (SLN)	(1)(0.5)	(Al,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Si, Sn,Ta,Ti,V,W,Zr)(B,C,H,N,O,Va)
HfTaO	CEF (SLN)	(6)(1)	(HfO2,Ta2O5)(HfO2,Ta2O5)
L10_TiAl	CEF (SLN)	(1)(1)(2)	(Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,V,W,Zr) (Al,Cr,Mn,Mo,Nb,Sn,Ta,Ti,V,W,Zr) (C,O,N,Va)
L12_(Al,Mn)3Ti	CEF (SLN)	(0.25)(0.08) (0.67)	(Al,Mn,Ti)(Al,Mn)(Al,Mn,Ti)
L12_Ni3Si	CEF (SLN)	(0.75)(0.25)(1)	(Ni,Si)(Ni,Si)(Va)
Laves_C14	CEF (SLN)	(2)(1)	(Al,Cr,Fe,Mn,Mo,Nb,Si,Ta,Ti,V,Zr) (Al,Cr,Fe,Mn,Mo,Nb,Ta,Ti,V,W,Zr)
Laves_C15	CEF (SLN)	(2)(1)	(Al,Cr,Mo,Mn,Nb,Si,Ta,Ti,V,W,Zr) (Al,Cr,Mo,Mn,Nb,Si,Ta,Ti,V,Zr)
Laves_C36	CEF (SLN)	(2)(1)	(Al,Cr,Ni,Ti,V,Zr)(Al,Cr,Ni,Ti,V,Zr)
Liquid	CEF (SLN)	(1)	(Al,B,C,Cr,Cu,Fe,H,Hf,Mn,Mo,N, Nb,Ni,O,Si,Sn,Ta,Ti,V,W,Zr,Al2O3, Cr2O3,CuO,Cu2O,Cu2O3,FeO, HfO2,MoO2,MoO3,NbO,NbO2, Nb2O5,NiO,Si3N4,SiO2,SnO, SnO2,Ta2O5,WO2,WO3,Zr1/2O)

Name	Model	Lattice Size	Constituent
M23C6	CEF (SLN)	(20)(3)(6)	(Cr,Mn,Mo,Ni)(Cr,Mn,Mo,Ni,W)(C)
M2B	CEF (SLN)	(2)(1)	(Cr,Fe,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 (SLN)	(3)(4)	(Cr,Fe)(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,Ni,W)(C)
MB2	CEF (SLN)	(1)(2)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,Zr,Va)(B,C,Va)
MH2_Delta	CEF (SLN)	(1)(2)	(Hf,Nb,Ti,Zr)(H,Va)
MH2_Eps	CEF (SLN)	(1)(2)	(Zr)(H,Va)
MO2	CEF (SLN)	(1)(2)	(Hf,Mo,W,Zr)(O)
MSi2	CEF (SLN)	(1)(2)	(Mo,Nb,W)(Si,Va)
Mn11Si19	CEF (ST2)	(11)(19)	(Mn)(Si)
Mn19Sn6	CEF (ST2)	(19)(6)	(Mn)(Sn)
Mn23C6	CEF (ST2)	(23)(6)	(Mn)(C)
Mn2Sn	CEF (ST2)	(2)(1)	(Mn)(Sn)
Mn2Zr	CEF (SLN)	(2)(1)	(Mn)(Zr,Va)
Mn3B4	CEF (ST2)	(0.428571) (0.571429)	(Mn)(B)
Mn3C	CEF (ST2)	(3)(1)	(Mn)(C)
Mn3Si	CEF (ST2)	(3)(1)	(Mn)(Si)
Mn3Ti	CEF (ST2)	(3)(1)	(Mn)(Ti)

Name	Model	Lattice Size	Constituent
Mn4Ti	CEF (SLN)	(0.815)(0.185)	(Mn,V)(Ti)
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 (ST2)	(17)(3)	(Mn)(Si)
Mn7C3	CEF (ST2)	(7)(3)	(Mn)(C)
Mn9Si2	CEF (ST2)	(33)(7)	(Mn)(Si)
MnB	CEF (ST2)	(1)(1)	(Mn)(B)
MnB2	CEF (ST2)	(0.333333) (0.666667)	(Mn)(B)
MnB4	CEF (ST2)	(0.2)(0.8)	(Mn)(B)
MnNi	CEF (SLN)	(1)(1)	(Mn,Ni)(Mn,Va)
MnNi2	CEF (SLN)	(1)(2)	(Mn,Ni)(Ni)
MnNi3	CEF (SLN)	(0.75)(0.25)	(Mn,Ni)(Mn,Ni)
MnNi_Beta	CEF (SLN)	(1)(1)	(Mn,Ni)(Mn,Ni)
MnSi	CEF (ST2)	(1)(1)	(Mn)(Si)
MnSn2	CEF (ST2)	(1)(2)	(Mn)(Sn)
Mo2B5	CEF (SLN)	(2)(5)	(Mo)(B,Va)
Mo3Sn	CEF (ST2)	(3)(1)	(Mo)(Sn)
Mo4O11	CEF (ST2)	(0.266667) (0.733333)	(Mo)(O)
Mo8O23	CEF (ST2)	(0.258064) (0.741935)	(Mo)(O)
Mo9O26	CEF (ST2)	(0.257143) (0.742857)	(Mo)(O)
MoB4	CEF (ST2)	(0.8)(0.2)	(B)(Mo)
MoC_Eta	CEF (SLN)	(1)(1)	(Mo,Ti)(C,Va)

Name	Model	Lattice Size	Constituent
MoC_shp	CEF (ST2)	(1)(1)	(Mo)(C)
MoNi	CEF (SLN)	(0.428571) (0.357143) (0.214286)	(Ni)(Mo,Ni)(Mo)
MoNi3	CEF (SLN)	(0.75)(0.25)	(Mo,Ni)(Mo,Ni)
MoNi4	CEF (ST2)	(0.2)(0.8)	(Mo)(Ni)
MoO3	CEF (ST2)	(1)(3)	(Mo)(O)
MoSn	CEF (ST2)	(1)(1)	(Mo)(Sn)
MoSn2	CEF (ST2)	(1)(2)	(Mo)(Sn)
Mu_Phase	CEF (SLN)	(7)(2)(4)	(Fe,Mn,Mo,Nb,Ni,Ta)(Mo,Nb,Ni,Ta,W) (Fe,Mo,Nb,Ni,Ta,W)
Nb2B3	CEF (ST2)	(2)(3)	(Nb)(B)
Nb2O5	CEF (ST2)	(2)(5)	(Nb)(O)
Nb3Si	CEF (ST2)	(0.75)(0.25)	(Nb)(Si)
Nb3Sn	CEF (SLN)	(3)(1)	(Nb,Sn)(Nb,Sn)
Nb5B6	CEF (SLN)	(5)(6)	(Nb,Ti)(B)
Nb5Si3_alpha	CEF (SLN)	(0.625)(0.375)	(Nb,Si)(Si)
Nb5Si3_beta	CEF (SLN)	(0.5)(0.125) (0.375)	(Nb)(Nb,Si)(Nb,Si)
Nb6Sn5	CEF (SLN)	(24)(16)(4)	(Nb)(Sn)(Nb,Sn)
Nb7Ni6	CEF (SLN)	(1)(4)(2)(6)	(Nb,Ni)(Nb)(Nb,Ni)(Nb,Ni)
NbB	CEF (SLN)	(0.5)(0.5)	(Nb)(B,Va)
NbH	CEF (SLN)	(1)(0.85)	(Nb)(H,Va)
NbNi3	CEF (SLN)	(3)(1)	(Nb,Ni)(Nb,Ni)
NbNi8	CEF (ST2)	(8)(1)	(Ni)(Nb)
NbO	CEF (ST2)	(1)(1)	(Nb)(O)

Name	Model	Lattice Size	Constituent
NbO2	CEF (ST2)	(1)(2)	(Nb)(O)
NbSi2	CEF (SLN)	(0.333)(0.667)	(Nb,Si)(Si)
NbSn2	CEF (ST2)	(1)(2)	(Nb)(Sn)
Ni10Zr7	CEF (ST2)	(10)(7)	(Ni)(Zr)
Ni11Zr9	CEF (ST2)	(11)(9)	(Ni)(Zr)
Ni21Zr8	CEF (ST2)	(21)(8)	(Ni)(Zr)
Ni2B	CEF (ST2)	(0.667)(0.333)	(Ni)(B)
Ni2Cr	CEF (ST2)	(2)(1)	(Ni)(Cr)
Ni2SnTi	CEF (ST3)	(0.5)(0.25) (0.25)	(Ni)(Sn)(Ti)
Ni2Ta	CEF (SLN)	(2)(1)	(Ni,Ta)(Ni,Ta)
Ni2V	CEF (ST2)	(0.6667) (0.3333)	(Ni)(V)
Ni3Al	CEF (SLN)	(0.75)(0.25)	(Al,Ni,Ti)(Al,Ni,Ti)
Ni3B	CEF (ST2)	(3)(1)	(Ni)(B)
Ni3Sn2	CEF (SLN)	(0.5)(0.25) (0.25)	(Ni,Sn)(Ni)(Ni)
Ni3Sn4	CEF (SLN)	(0.4286) (0.5714)	(Ni)(Ni,Sn)
Ni3Sn_H	CEF (SLN)	(0.75)(0.25)	(Ni,Sn)(Ni,Sn)
Ni3Sn_L	CEF (SLN)	(0.75)(0.25)	(Ni,Sn)(Ni,Sn)
Ni3Ta	CEF (SLN)	(3)(1)	(Ni,Ta)(Ni,Ta)
Ni3Ta_L	CEF (ST2)	(0.75)(0.25)	(Ni)(Ta)
Ni3Ti	CEF (SLN)	(0.75)(0.25)	(Ni,Ti)(Ni,Ti)
Ni3V	CEF (SLN)	(3)(1)	(Ni,V)(Ni,V)
Ni3Zr	CEF (ST2)	(3)(1)	(Ni)(Zr)

Name	Model	Lattice Size	Constituent
Ni4W	CEF (ST2)	(4)(1)	(Ni)(W)
Ni5Zr	CEF (SLN)	(5)(1)	(Ni,Zr)(Zr,Va)
Ni7Zr2	CEF (ST2)	(7)(2)	(Ni)(Zr)
Ni8Ta	CEF (ST2)	(8)(1)	(Ni)(Ta)
NiB	CEF (ST2)	(0.5)(0.5)	(Ni)(B)
NiSi	CEF (ST2)	(1)(1)	(Ni)(Si)
NiSi2	CEF (ST2)	(1)(2)	(Ni)(Si)
NiSnTi	CEF (ST3)	(0.33333) (0.33333) (0.33334)	(Ni)(Sn)(Ti)
NiTa2	CEF (SLN)	(1)(2)	(Ni,Ta)(Ni,Ta)
NiTi2	CEF (SLN)	(1)(2)	(Ni,Cu)(Ti)
NiV3	CEF (ST2)	(0.25)(0.75)	(Ni)(V)
NiW	CEF (ST2)	(1)(1)	(Ni)(W)
NiW2	CEF (ST2)	(1)(2)	(Ni)(W)
NiZr	CEF (ST2)	(1)(1)	(Ni)(Zr)
NiZr2	CEF (ST2)	(1)(2)	(Ni)(Zr)
Phi	CEF (SLN)	(0.8837) (1.1163)	(Al,Ta,Ti)(Al,Ta,Ti)
Quartz	CEF (ST2)	(1)(2)	(Si)(O)
R_Phase	CEF (SLN)	(27)(14)(12)	(Fe)(Mo)(Fe,Mo)
Rutile	CEF (SLN)	(1)(2)	(Mn,Sn,Ti,V)(O)
Shp_MC	CEF (ST2)	(1)(1)	(W)(C)
Si2Zr	CEF (ST2)	(2)(1)	(Si)(Zr)
Si2Zr3	CEF (ST2)	(2)(3)	(Si)(Zr)

Name	Model	Lattice Size	Constituent
Si3N4	CEF (ST2)	(3)(4)	(Si)(N)
Si3V5	CEF (ST2)	(0.375)(0.625)	(Si)(V)
Si5V6	CEF (ST2)	(0.454545) (0.545455)	(Si)(V)
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 (ST2)	(1)(1)	(C)(Si)
SiZr2	CEF (SLN)	(1)(2)	(Si)(Ta,Zr)
Sigma	CEF (SLN)	(8)(4)(18)	(Al,Fe,Mn,Ni,Ta)(Cr,Mo,Nb,Ta,Ti,V) (Al,Cr,Fe,Mn,Mo,Nb,Ni,Ta,Ti,V)
Sn2V	CEF (ST2)	(2)(1)	(Sn)(V)
Sn2Zr	CEF (ST2)	(2)(1)	(Sn)(Zr)
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)
SnZr4	CEF (SLN)	(3)(1)	(Sn,Zr)(Sn,Zr)
T2	CEF (ST2)	(4)(3)	(Cr)(Si)
Ta2O5_S	CEF (SLN)	(1)	(Ta,Ta2O5)
Ta2O5_S2	CEF (SLN)	(1)	(Hf,Ta,Ta2O5)
Ta2Si	CEF (ST2)	(2)(1)	(Ta)(Si)
Ta3Si	CEF (ST2)	(3)(1)	(Ta)(Si)
TaSi2	CEF (ST2)	(1)(2)	(Ta)(Si)

Name	Model	Lattice Size	Constituent
Theta_Ni2Si	CEF (SLN)	(1)(1)(1)	(Ni)(Ni,Va)(Si)
Ti2AlN	CEF (ST3)	(2)(1)(0.82)	(Ti)(Al)(N)
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)
Ti3B4	CEF (ST2)	(4)(3)	(B)(Ti)
Ti3N2	CEF (ST2)	(0.71)(0.29)	(Ti)(N)
Ti3O2	CEF (ST2)	(3)(2)	(Ti)(O)
Ti3SiC2	CEF (ST3)	(3)(1)(2)	(Ti)(Si)(C)
Ti4N3	CEF (ST2)	(0.685)(0.315)	(Ti)(N)
Ti5Al11	CEF (ST2)	(17)(8)	(Al)(Ti)
TiAl2	CEF (SLN)	(2)(1)	(Al)(Nb,Ti)
TiB	CEF (ST2)	(1)(1)	(B)(Ti)
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)
V2Zr	CEF (ST2)	(2)(1)	(V)(Zr)
V3B2	CEF (ST2)	(3)(2)	(V)(B)
V3B4	CEF (ST2)	(3)(4)	(V)(B)
V3Sn	CEF (SLN)	(0.25)(0.75)	(Sn,V)(V)
V5B6	CEF (ST2)	(5)(6)	(V)(B)
VB	CEF (ST2)	(1)(1)	(V)(B)
VB2	CEF (ST2)	(1)(2)	(V)(B)

Name	Model	Lattice Size	Constituent
W2B	CEF (ST2)	(2)(1)	(W)(B)
W2B5	CEF (SLN)	(2)(5)	(W)(B,Va)
W2B9	CEF (ST2)	(2)(9)	(W)(B)
WO272	CEF (ST2)	(1)(2.72)	(W)(O)
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)	(Hf,Zr)(O,Va)
ZrO2_Tetra-gonal	CEF (SLN)	(1)(2)	(Hf,Zr)(O,Va)
m_Ni4B3	CEF (ST2)	(0.564)(0.436)	(Ni)(B)
o_Ni4B3	CEF (ST2)	(0.586)(0.414)	(Ni)(B)