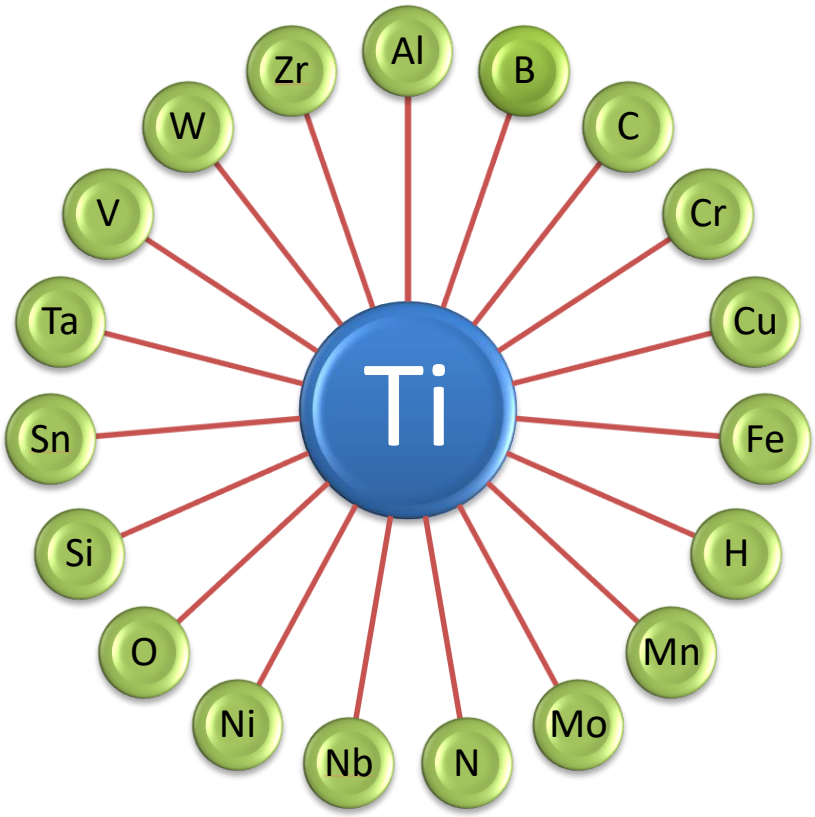
1. PanTitanium

Thermodynamic Database for Titanium-Based Alloys



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1.1 Components

A total of 20 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, 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 1.5.

Table 1.1: Suggested composition range

Element	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, Mn, Si	0-0.5

1.3 Phases

A total of 320 phases are included in the current database, and Table 1.2 lists those that are important for commercial titanium alloys. Information on all the other phases may be displayed through TDB viewer in Pandat software and can be found at www.computherm.com.

Table 1.2: Phase 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,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,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,Mn,Mo,N,Nb,Ni,O,Si,Sn,Ta, Ti,V,W,Zr,Al2O3,Cr2O3,FeO,MoO2,MoO3,NbO, NbO2,Nb2O5,NiO,Si3N4,SiO2)
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 Sub-System Information

The composition limits given in Table 1.1 are for multicomponent commercial titanium alloys in general. Complete and partial thermodynamic descriptions are developed for many binary systems as listed in Table 1.3. Thermodynamic descriptions are fully developed for the binaries in green color, which means

that there is no composition limits if calculations are carried out for these binary systems. Only major phases are considered for the binaries in yellow color. For these binaries, phase relationships are correct in the areas near the major phases. No model parameters are developed for those binaries in white color.

Thermodynamic description for the key ternary systems are also developed and listed in Table 1.4 in which the colors represent the same modeling status as those in Table 1.3.

: Full description

: Full description for major phases

: Partial description in Ti-rich corner

: Extrapolation

Table 1.3: Current Status of Key Binary Systems

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

Table 1.4: Current Status of Key Ternary Systems

Ti-Al-Cr	Ti-Al-Fe	Ti-Al-Mn	Ti-Al-Mo	Ti-Al-Nb	Ti-Al-Ni	Ti-Al-Si	Ti-Al-V
Ti-Cr-Mn	Al-Cr-Nb						
Ti-Cr-Fe	Cr-Ti-V	Ti-Nb-Zr	Ti-Al-Sn	Ti-Al-Zr			
Ti-Al-O	Ti-Al-N	Ti-Al-C	Ti-Al-H	Ti-V-O	Ti-V-N	Ti-V-C	Ti-V-H
Ti-Cr-O	Ti-Cr-N	Ti-Cr-C	Ti-Cr-H	Ti-Fe-O	Ti-Fe-N	Ti-Fe-C	Ti-Fe-H
Ti-Mn-O	Ti-Mn-N	Ti-Mn-C	Ti-Mn-H	Ti-Mo-O	Ti-Mo-N	Ti-Mo-C	Ti-Mo-H
Ti-Nb-O	Ti-Nb-N	Ti-Nb-C	Ti-Nb-H	Ti-Ni-O	Ti-Ni-N	Ti-Ni-C	Ti-Ni-H
Ti-Si-O	Ti-Si-N	Ti-Si-C	Ti-Si-H				

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 1.5 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 1.5: 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	[2003Ven]

	partition coefficient	
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]
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.

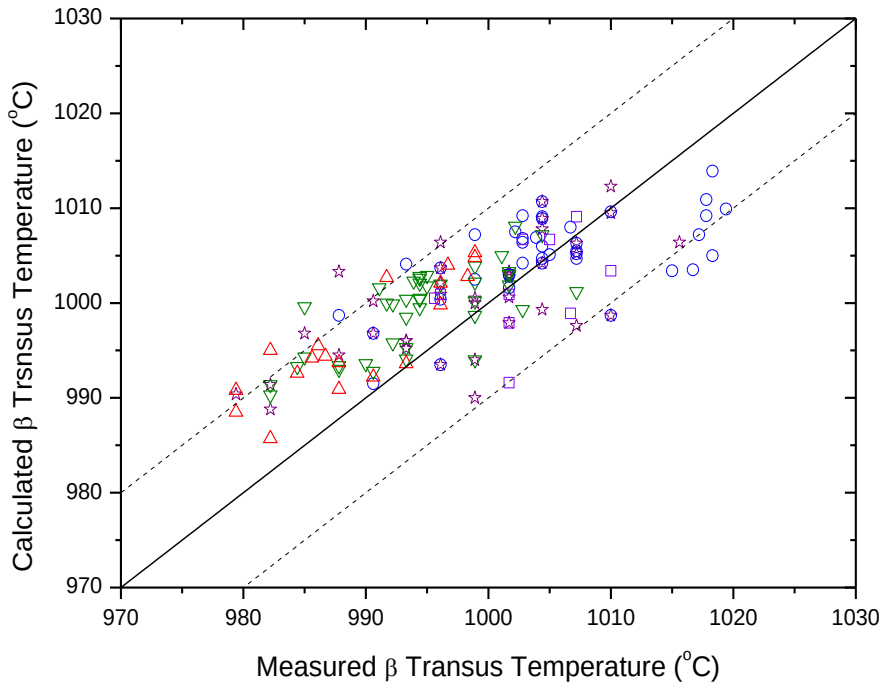

Figure 1.1: Comparison between the predicted and observed beta transus for more than 150 Ti64 heats. The calculated transformation temperatures correspond to 0% of α phase formed and the experimental data are from [1966Cas, 2003Sem, 2003Fur].

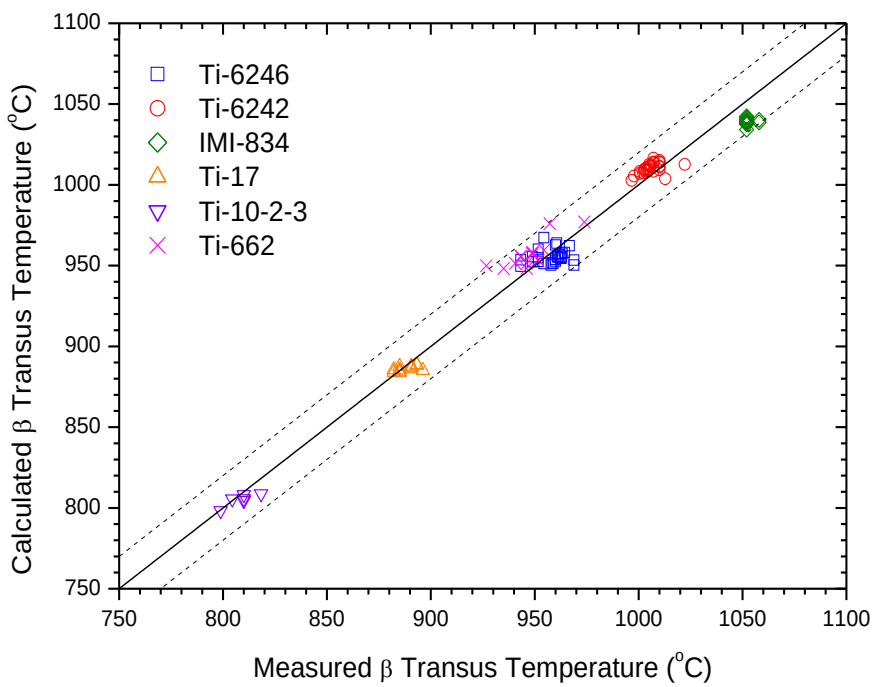

Figure 1.2: Comparison between the predicted and observed beta transus for other titanium alloys. The calculated transformation temperatures correspond to 0% of α phase formed.

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.

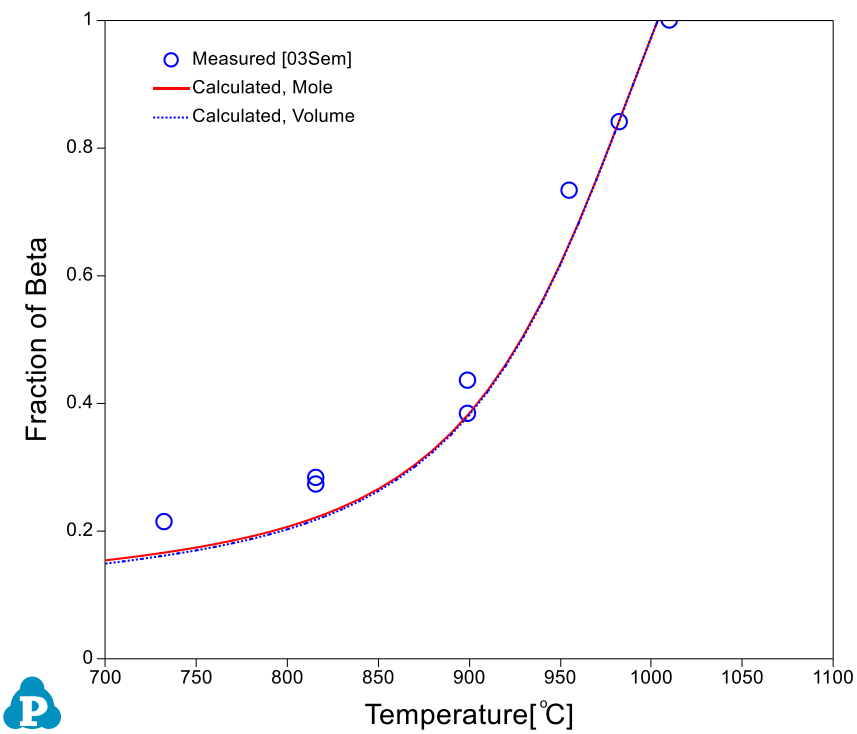

Figure 1.3: Beta approach curve for a Ti64 alloy with experimental data from [2003Sem].

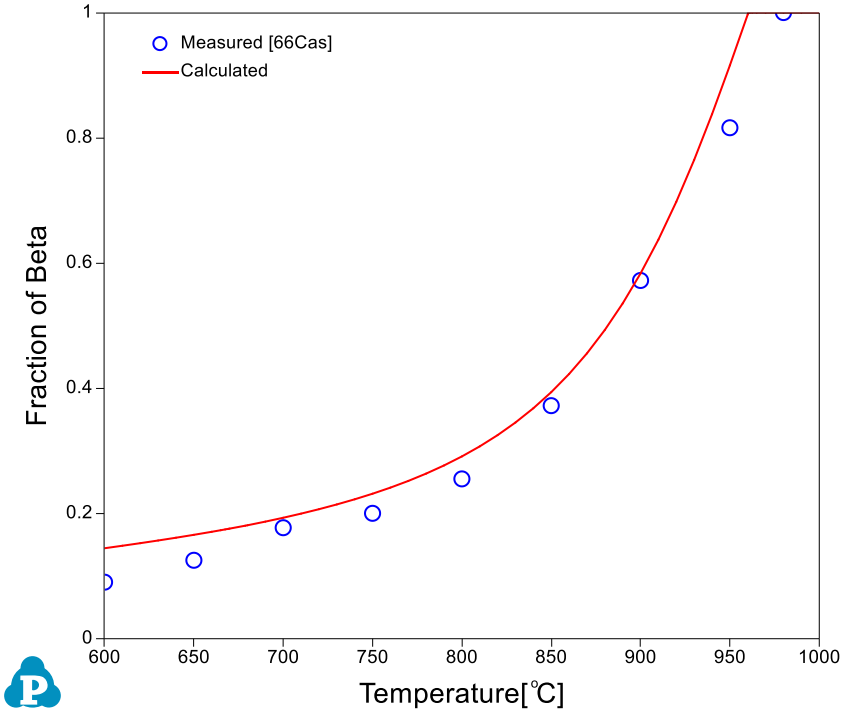

Figure 1.4: Beta approach curve for a Ti64 alloy with experimental data from [1966Cas].

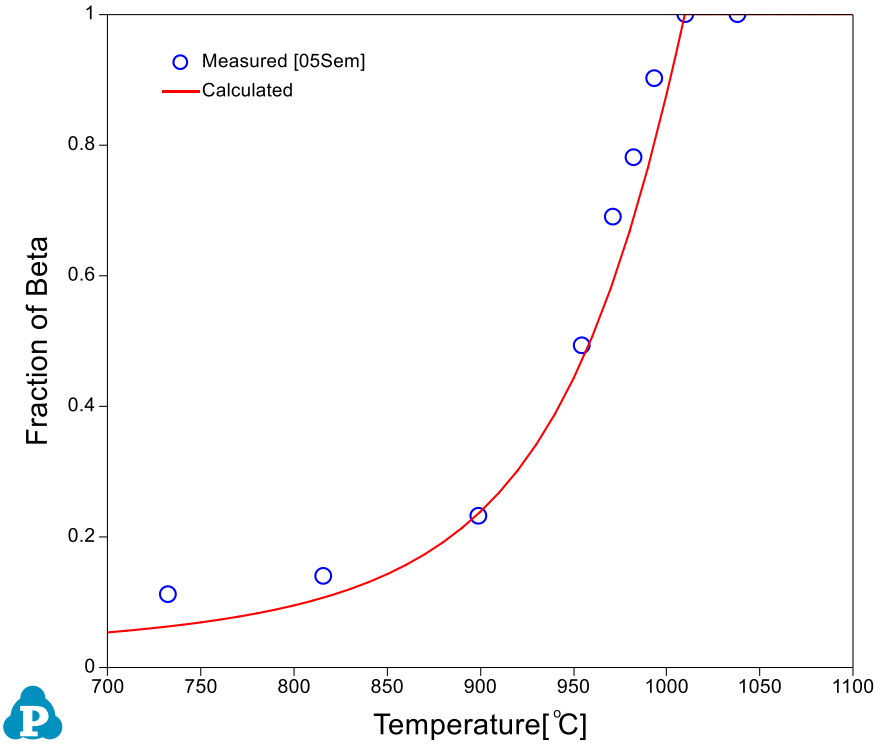

Figure 1.5: Beta approach curve for a Ti-6242 alloy with experimental data from [2005Sem].

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.

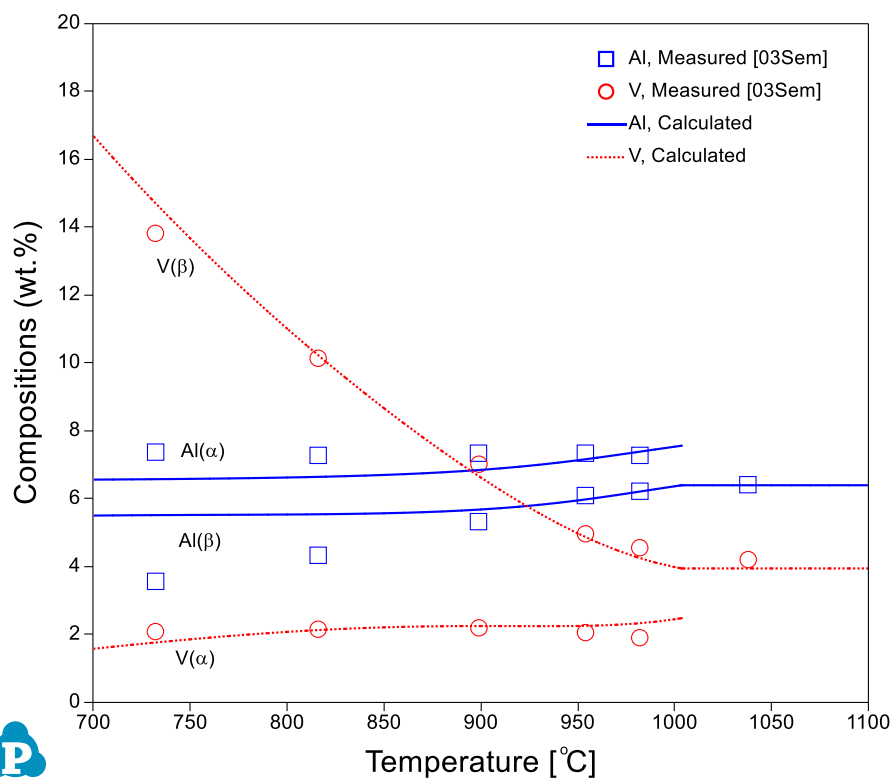

Figure 1.6: Equilibrium compositions of Al and V in the α and β phases for a Ti64 alloy with the experimental data from [2003Sem].

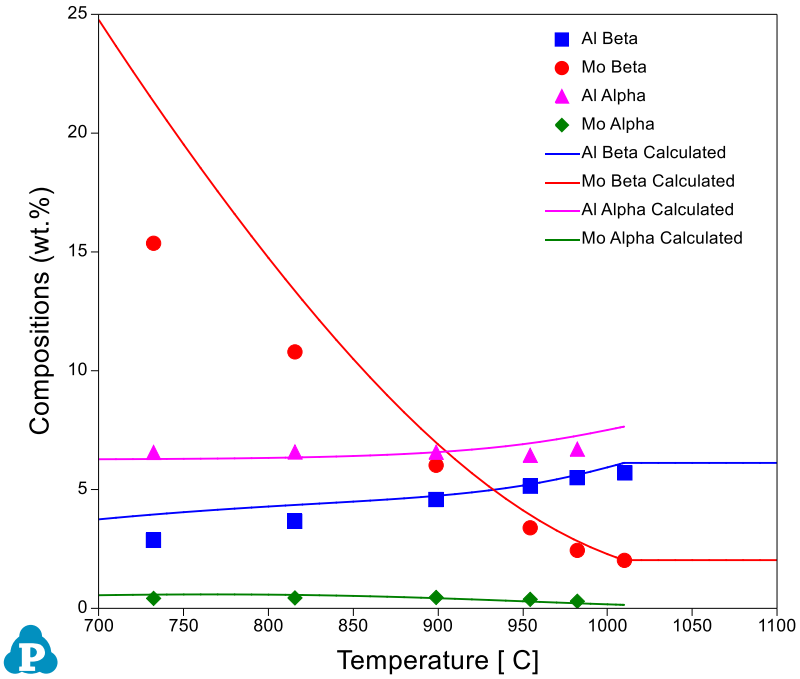

Figure 1.7： Equilibrium compositions of Al and Mo in the alpha and beta phases for a Ti6242 alloy with the experimental data from [2005Sem].

Figure 1.8 ~ 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.

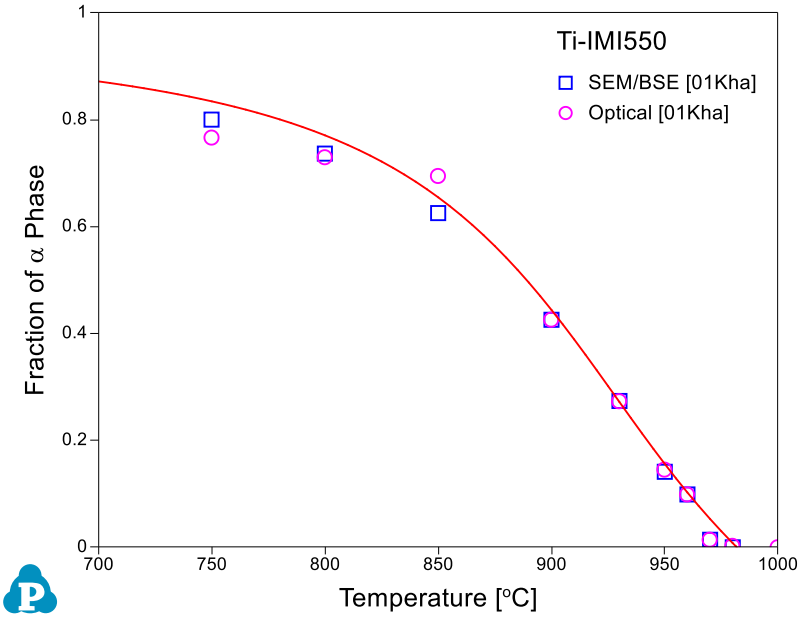

Figure 1.8：Alpha fraction curve for an IMI550 alloy with experimental data [2001Kha].

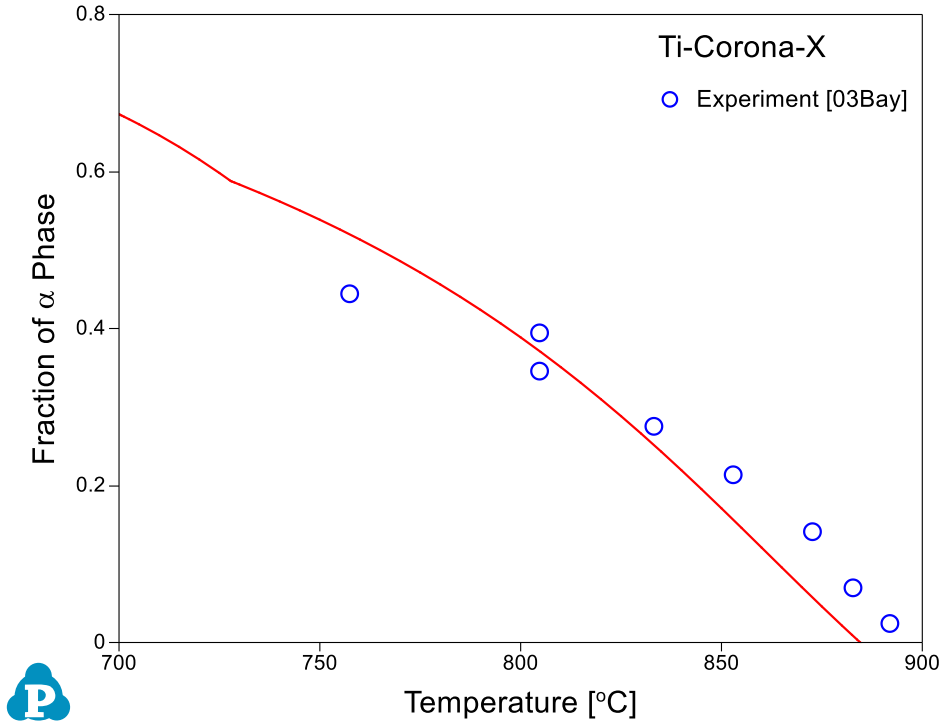

Figure 1.9： Alpha fraction curve for a Corona-X alloy with experimental data [2001Kha].

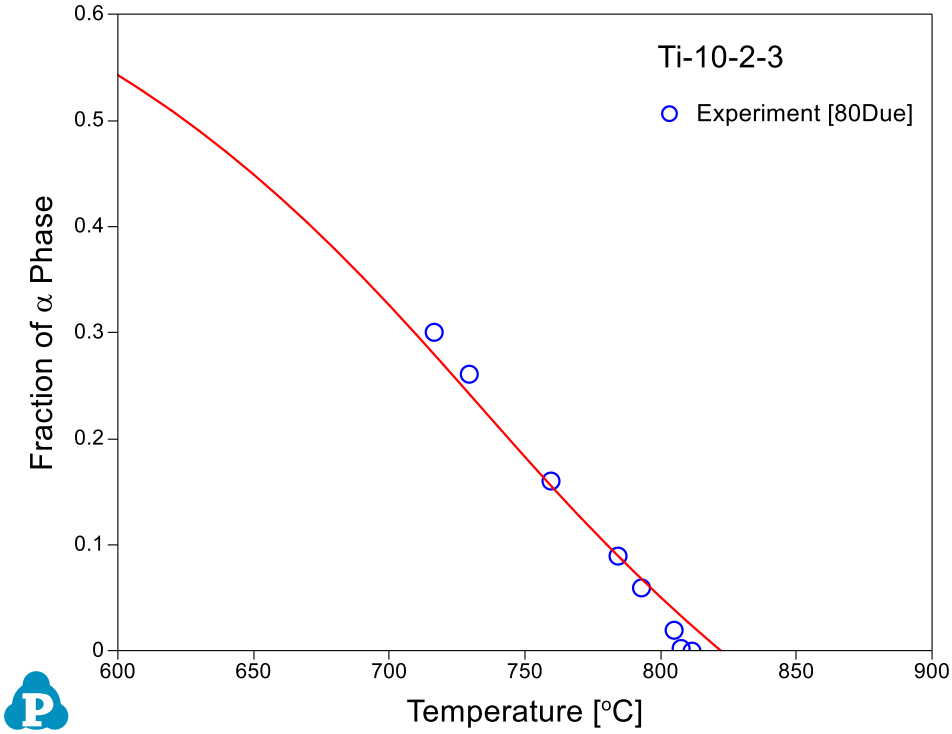

Figure 1.10：Alpha fraction curve for a Ti-10-2-3 alloy with experimental data [1980Due].

1.6 References

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