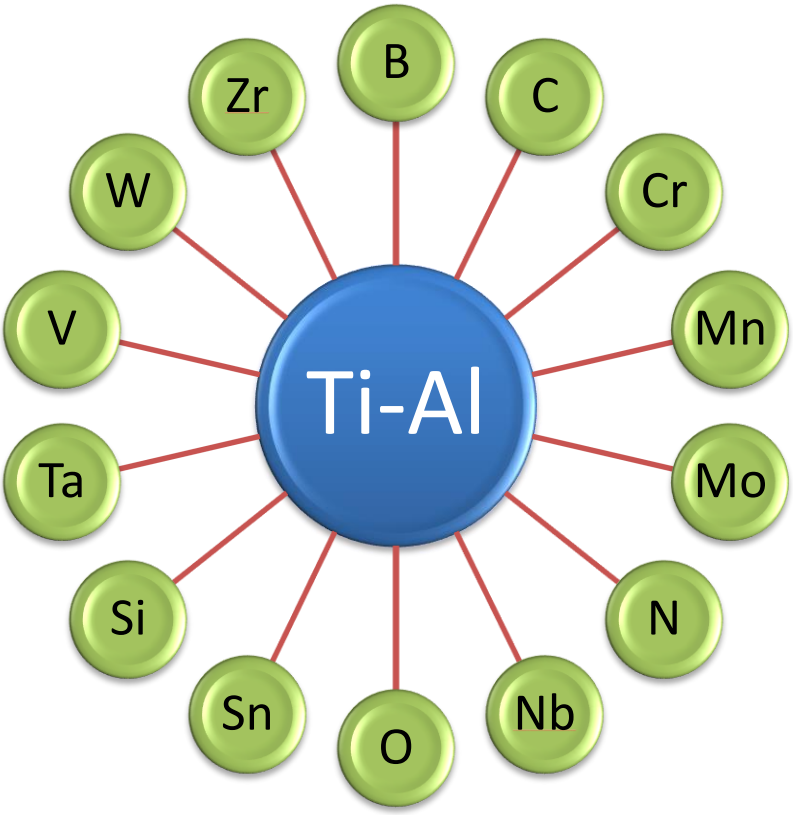
1. PanTiAl

Thermodynamic Database for TiAl-Based Alloys



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1.1 Components

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 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

Element	Composition range (wt%)
Ti	50-100
Al	0-35
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 184 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 of Pandat and can be found at www.computherm.com.

Table 1.2: Phase Information

Name	Model	Lattice Size	Constituent
A15	CEF	(3)(1)	(Al,Cr,Mo,Nb,Ta,Ti)(Al,Mo,Nb,Sn,Ti)
B2	CEF	(1)(1)	(Al,Cr,Mn,Mo,Nb,Ti)(Cr,Mn,Mo,Nb,Ti,Va)
Bcc	CEF	(1)(3)	(Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,V,W,Zr) (B,C,N,O,Va)
Bcc_B2	CEF	(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	CEF	(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	(0.75)(0.25)(0.5)	(Al,Cr,Mo,Si,Ti)(Al,Cr,Mo,Nb,Ta,Ti,V) (C,Va)
Fcc	CEF	(1)(1)	(Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,V,W,Zr) (B,C,N,O,Va)
Hcp	CEF	(1)(0.5)	(Al,Cr,Mn,Mo,Nb,Si,Sn,Ta,Ti,V,W,Zr) (B,C,N,O,Va)
L10_TiAl	CEF	(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	CEF	(2)(1)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,V,Zr) (Al,Cr,Mn,Mo,Nb,Ta,Ti,V,Zr)
Laves_C15	CEF	(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	(2)(1)	(Al,Cr,Ti,V,Zr)(Al,Cr,Ti,V,Zr)
Liquid	CEF	(1)	(Al,B,C,Cr,Mn,Mo,N,Nb,O,Si,Sn,Ta,Ti,V, W,Zr,Al2O3,Cr2O3,NbO,NbO2,Nb2O5, SiO2)
Mu	CEF	(7)(2)(4)	(Al,Cr,Mn,Mo,Nb)(Mo,Nb,Ti)(Cr,Mo,Nb,Ti)
Sigma	CEF	(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 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. This means the current database works in a much wider composition range in many sub-systems.

Table 1.3 lists all the binaries in the 16-component system. 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. The color represents the following meaning:

: Full description

: Full description for major phases

: Extrapolation

Table 1.3: Current Status of All Binary Systems

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

In addition to the binaries, thermodynamic descriptions for the key ternary systems Ti-Al-X (X=Cr, Mn, Mo, Nb, Si, V, W) are also developed.

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 1.4 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 1.4: Comparison between the calculated α transus (α=>γ) temperatures and experimentally determined ones

Alloy Composition (at.%)	Determined T(ºC)	Calculated T(ºC)	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]
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]

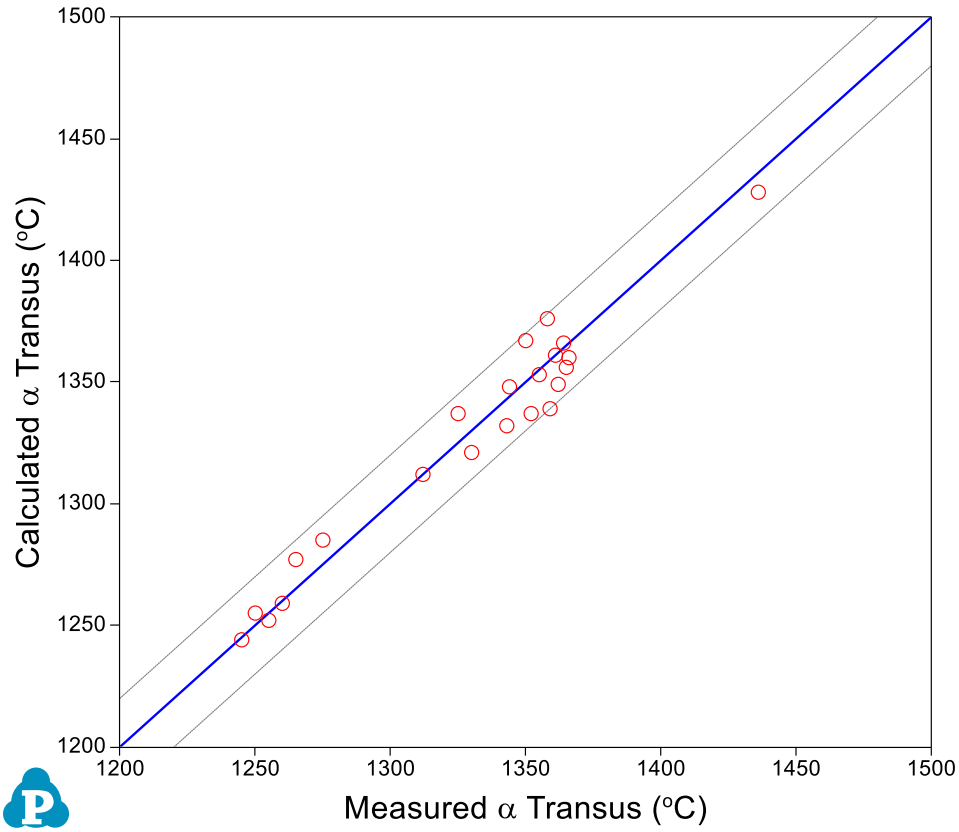

Figure 1.1: Comparison between calculated and measured α transus temperatures [1992Lom, 1993Fuc, 1995Bho, 1995Fuc, 1995Kim, 2014Pen].

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 experimental data indicate that 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.

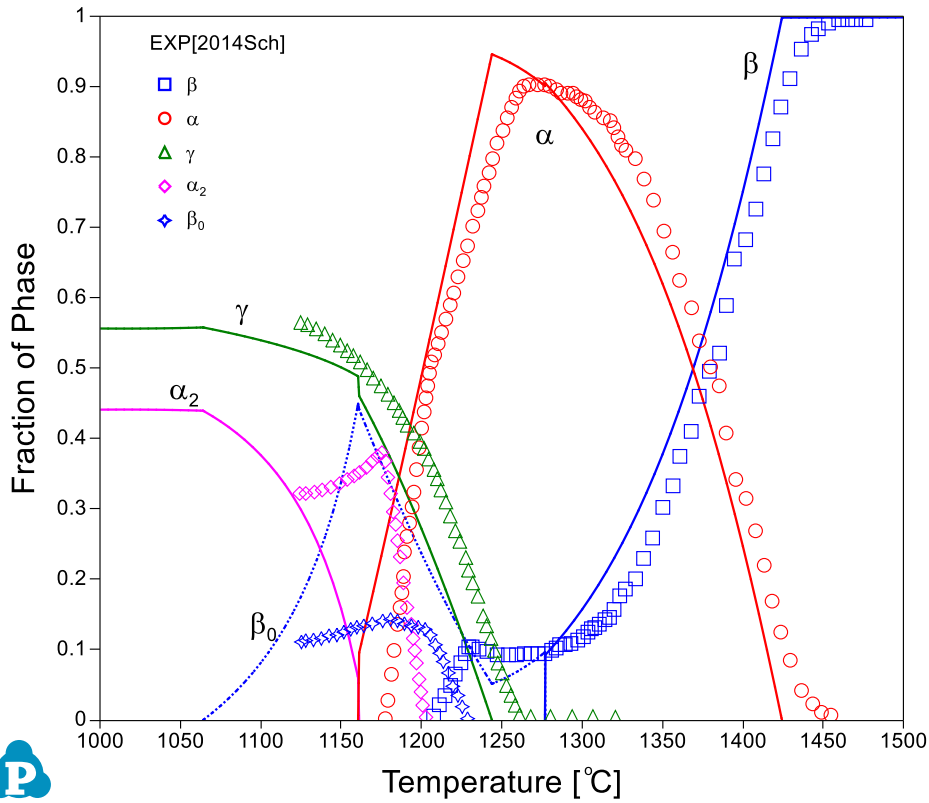

Figure 1.2: Calculated phase fractions for alloy Ti-43Al-4Nb-1Mo-0.1B (in at.%) compared with experimental data [2014Sch]

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 1.5, 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 due to the slow cooling rate after aging. The calculations are in reasonable agreement with the experimental data.

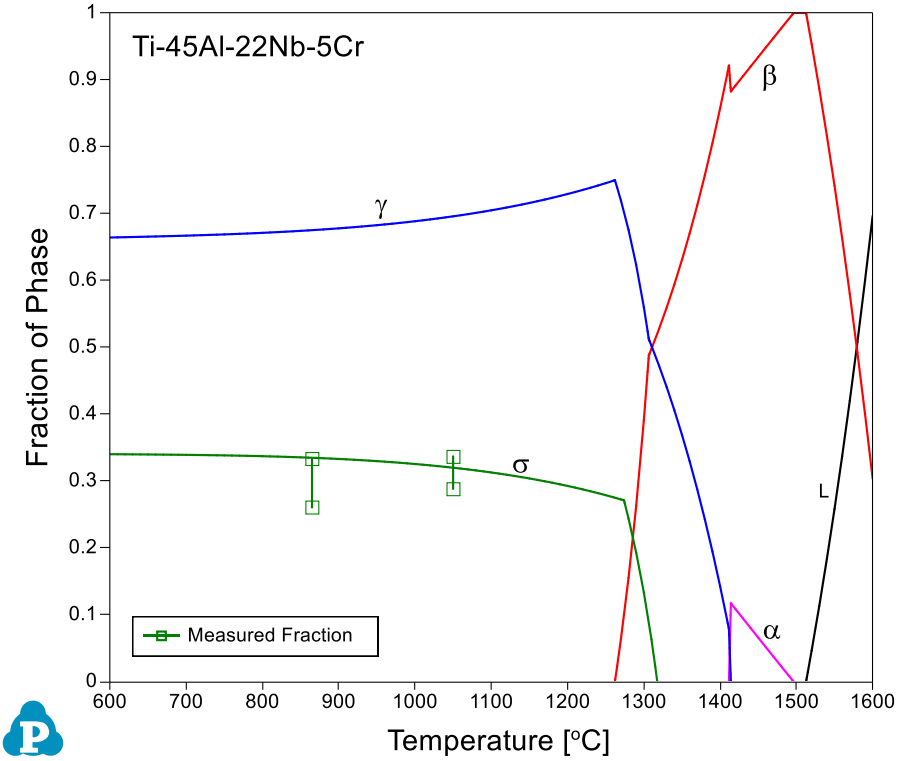

Figure 1.3: Calculated phase fractions for alloy Ti-45Al-22Nb-5Cr (in at.%) compared with experimental data [2011Kes]

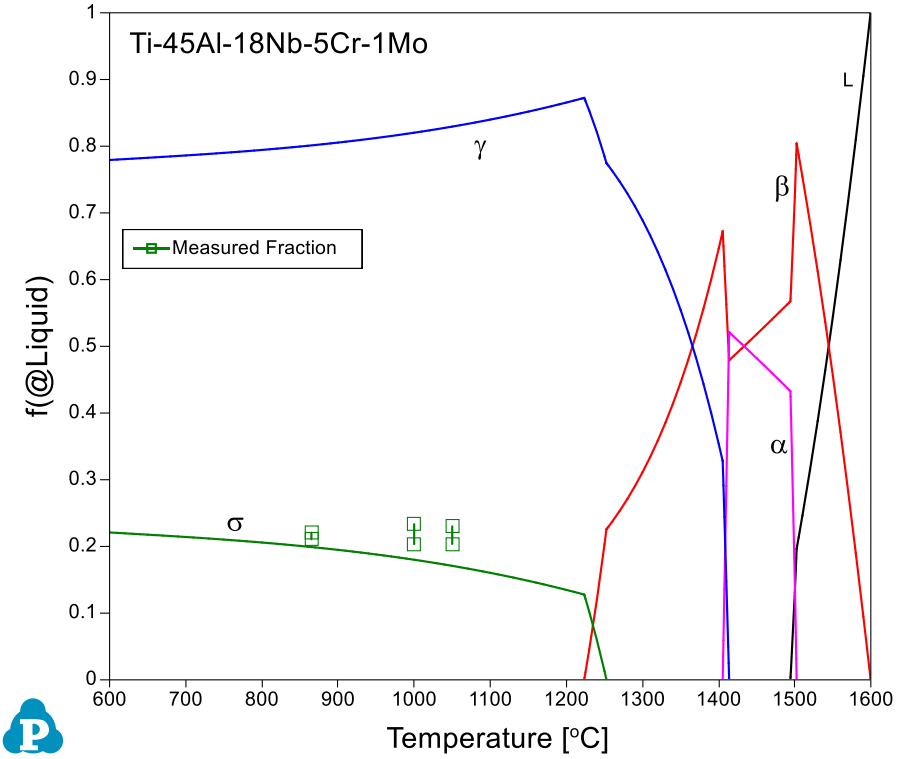

Figure 1.4: Calculated phase fractions for alloy Ti-45Al-18Nb-5Cr-1Mo (in at.%) compared with experimental data [2011Kes]

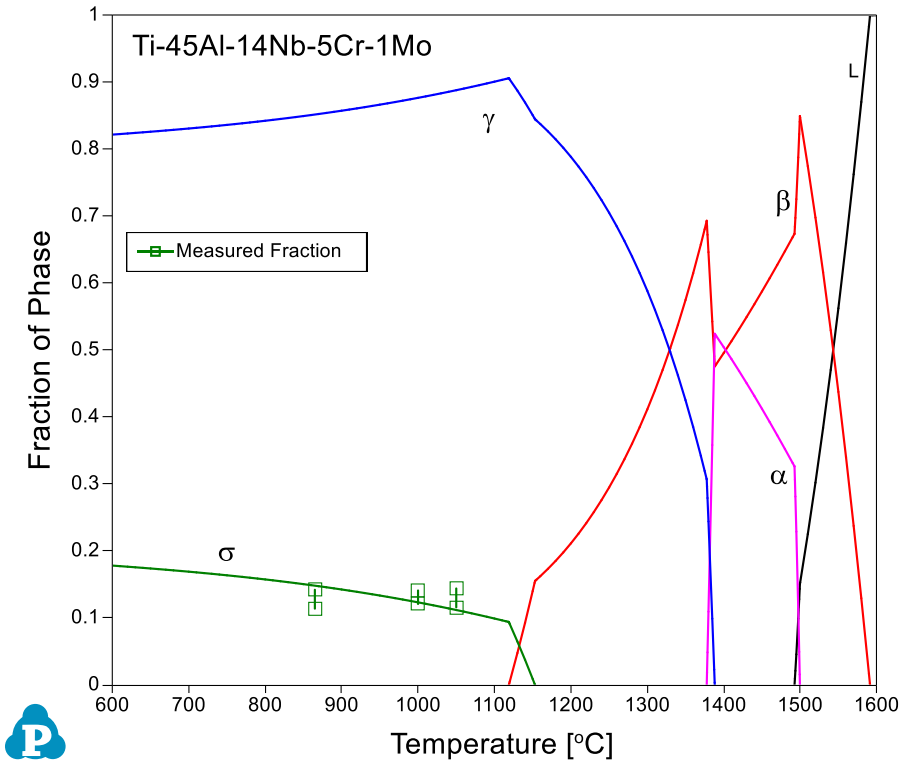

Figure 1.5: Calculated phase fractions for alloy Ti-45Al-14Nb-5Cr-1Mo (in at.%) compared with experimental data [2011Kes]

1.6 References

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