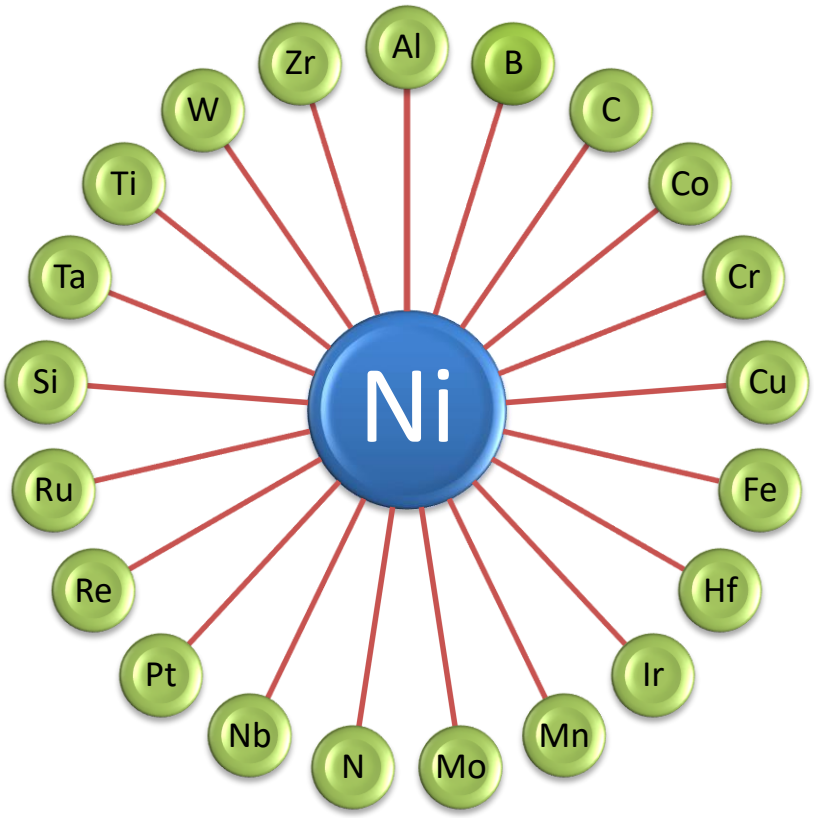
1. PanNickel

Thermodynamic Database for Nickel-Based Superalloys



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1.1 Components

A total of 22 components are included in the database as listed here:

Al-B-C-Co-Cr-Cu-Fe-Hf-Ir-Mn-Mo-N-Nb-**Ni**-Pt-Re-Ru-Si-Ta-Ti-W-Zr

1.2 Suggested Composition Range

The suggested composition range for each element is listed in Table 1.1. It should be noted that this composition range is based on the validation we performed on commercial alloys. For particular subsystems, the application range may be wider. Some subsystems can be applied to the entire composition range as given in Table 1.4.

Table 1.1: Suggested composition range

Element	Composition range (wt%)
Ni	50-100
Al,Co,Cr,Fe	0-22
Ir,Mo,Re,Ru,W	0-12
Hf,Nb,Ta,Ti	0-5
B,C,Cu,Mn,N,Si,Zr	0-0.5
Pt	0-40

1.3 What's new in PanNi2020

Model parameters for the γ' phase are significantly improved in PanNi2020 so that the γ' solvus temperatures and equilibrium phase fractions are more accurate for many commercial alloys. This improvement is important not only for phase equilibrium calculation, but also for precipitation simulation.

1.4 Phases

A total of 149 phases are included in the current database. The names and thermodynamic models of the major phases are given in Table 1.2. Information on all phases can be displayed in the TDB viewer of Pandat or can be found at www.computherm.com.

Table 1.2: Phase name and related information

Name	Lattice Size	Constituent
B2	(1)(1)	(Al,Co,Cr,Fe,Hf,Ir,Mn,Mo,Nb, Ni,Pt,Re,Ru,Si,Ta,Ti,W) (Al,Co,Cr,Fe,Hf,Ir,Mn,Mo,Nb, Ni,Pt,Re,Ru,Si,Ta,Ti,W,Va)
Bcc	(1)(3)	(Al,Co,Cr,Cu,Fe,Hf,Ir,Mn,Mo,Nb, Ni,Pt,Re,Ru,Si,Ta,Ti,W,Zr) (B,C,N,Va)
Chi_A12	(24)(10)(24)	(Cr,Fe,Ni,Re)(Cr,Mo,Ta,W) (Cr,Fe,Mo,Ni,Re,Ta,W)
Delta	(3)(1)	(Al,Co,Cr,Fe,Mo,Nb,Ni,Re,Ta,Ti) (Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Ta,Ti,W)
Eta	(0.75)(0.25)	(Co,Fe,Ni,Ti)(Al,Cr,Hf,Mo,Nb,Ni,Ta,Ti)
Fcc	(1)(1)	(Al,Co,Cr,Cu,Fe,Hf,Ir,Mn,Mo,Nb, Ni,Pt,Re,Ru,Si,Ta,Ti,W,Zr) (B,C,N,Va)
FCC_MC	(1)(1)	(Co,Cr,Hf,Mo,Nb,Ni,Si,Ta,Ti,W,Zr)(B,C,N,Va)
Hcp	(1)(0.5)	(Al,Co,Cr,Cu,Fe,Hf,Ir,Mo,Nb, Ni,Pt,Re,Ru,Si,Ta,Ti,W,Zr) (B,C,N,Va)
HCP_M2C	(1)(0.5)	(Co,Cr,Fe,Mo,Nb,Ni,Ta,Ti,W)(B,C,N,Va)
L12_FCC	(0.75)(0.25)(1)	(Al,Co,Cr,Fe,Hf,Ir,Mn,Mo,Nb, Ni,Pt,Re,Ru,Si,Ta,Ti,W,Zr) (Al,Co,Cr,Fe,Hf,Ir,Mn,Mo,Nb, Ni,Pt,Re,Ru,Si,Ta,Ti,W,Zr)(Va)
Laves_C14	(2)(1)	(Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Ta,Ti,W,Zr) (Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Ta,Ti,W,Zr)
Laves_C15	(2)(1)	(Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Ta,Ti,W,Zr)

		(Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Ta,Ti,W,Zr)
Liquid	(1)	(Al,B,C,Co,Cr,Cu,Fe,Hf,Ir,Mn,Mo, N,Nb,Ni,Pt,Re,Ru,Si,Ta,Ti,W,Zr)
M23C6	(20)(3)(6)	(Co,Cr,Fe,Ni,Re) (Co,Cr,Fe,Mo,Nb,Ni,Re,Ta,Ti,W)(B,C)
M2B	(2)(1)	(Co,Cr,Fe,Mo,Ni,Ta,W)(B)
M3B2	(2)(1)(2)	(Co,Cr,Fe,Mo,Nb,Ni,Ta,W) (Co,Cr,Fe,Nb,Ni,Ta,W)(B)
M3Si	(3)(1)	(Co,Cr,Fe,Mo,Nb,Ni,Ta,Ti,Zr)(Si)
M5Si3	(0.625)(0.375)	(Cr,Fe,Mo,Nb,Ta,Ti,W,Zr)(Si)
M6C	(2)(2)(2)(1)	(Co,Fe,Ni)(Cr,Mo,Nb,W) (Co,Cr,Fe,Mo,Nb,Ni,W)(C)
M7C3	(7)(3)	(Co,Cr,Fe,Mo,Nb,Ni,Re,W)(B,C)
MB2	(1)(2)	(Al,Cr,Hf,Mo,Nb,Re,Ta,Ti,Zr)(B)
MSi	(0.5)(0.5)	(Co,Cr,Fe,Hf,Nb,Ni,Ti,Zr)(Si)
Mu_Phase	(7)(2)(4)	(Co,Cr,Fe,Mo,Nb,Ni,Re,Ta) (Co,Cr,Mo,Nb,Ni,Re,Ta,Ti,W) (Co,Cr,Fe,Mo,Nb,Ni,Re,Ta,Ti,W)
NiMo	(24)(20)(12)	(Co,Cr,Fe,Ni,Re)(Al,Cr,Fe,Mo,Ni,Re,W)(Mo)
P_Phase	(24)(12)(20)	(Co,Cr,Fe,Ni,Re)(Mo,W) (Co,Cr,Fe,Mo,Ni,Re,W)
R_Phase	(27)(14)(12)	(Co,Cr,Fe,Ni)(Mo,W)(Co,Cr,Fe,Mo,Ni,W)
Sigma	(8)(4)(18)	(Al,Co,Fe,Mn,Ni,Re,Ru,Si) (Co,Cr,Mo,Nb,Ni,Ta,W) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Re,Ru,Si,Ta,W)
gamma_double _prime	(3)(1)	(Al,Co,Cr,Fe,Mo,Nb,Ni,Re,Ta,Ti) (Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Ta,Ti,W)

1.5 Key Elements and Subsystems

Table 1.3 lists major binaries and Table 1.4 lists the modeled ternaries in the 22-component system. Thermodynamic descriptions are fully developed for

the systems in green color, which means that there is no composition limits if calculations are carried out for these systems. Only major phases are considered for the systems in yellow color. For these systems, phase relationships are correct in the areas near the major phases. In the ternary systems with light blue color, only patial descriptions for major phases are developed, which means the descriptions are good within low concentration of boron or carbon. No model parameters are developed for those systems in white color.

: Full description

: Full description for major phases

: Partial description for major phases

: Extrapolation

Table 1.3: Current Status of Key Binary Systems

	Co	Cr	Fe	Hf	Ir	Mo	Nb	Ni	Pt	Re	Ru	Si	Ta	Ti	W	Zr
Al	Al-Co	Al-Cr	Al-Fe	Al-Hf	Al-Ir	Al-Mo	Al-Nb	Al-Ni	Al-Pt	Al-Re	Al-Ru	Al-Si	Al-Ta	Al-Ti	Al-W	Al-Zr
Co		Co-Cr	Co-Fe	Co-Hf	Co-Ir	Co-Mo	Co-Nb	Co-Ni	Co-Pt	Co-Re	Co-Ru	Co-Si	Co-Ta	Co-Ti	Co-W	Co-Zr
Cr			Cr-Fe	Cr-Hf	Cr-Ir	Cr-Mo	Cr-Nb	Cr-Ni	Cr-Pt	Cr-Re	Cr-Ru	Cr-Si	Cr-Ta	Cr-Ti	Cr-W	Cr-Zr
Fe				Fe-Hf	Fe-Ir	Fe-Mo	Fe-Nb	Fe-Ni	Fe-Pt	Fe-Re	Fe-Ru	Fe-Si	Fe-Ta	Fe-Ti	Fe-W	Fe-Zr
Hf					Hf-Ir	Hf-Mo	Hf-Nb	Hf-Ni	Hf-Pt	Hf-Re	Hf-Ru	Hf-Si	Hf-Ta	Hf-Ti	Hf-W	Hf-Zr
Ir						Ir-Mo	Ir-Nb	Ir-Ni	Ir-Pt	Ir-Re	Ir-Ru	Ir-S	Ir-Ta	Ir-Ti	Ir-W	Ir-Zr
Mo							Mo-Nb	Mo-Ni	Mo-Pt	Mo-Re	Mo-Ru	Mo-Si	Mo-Ta	Mo-Ti	Mo-W	Mo-Zr
Nb								Nb-Ni	Nb-Pt	Nb-Re	Nb-Ru	Nb-Si	Nb-Ta	Nb-Ti	Nb-W	Nb-Zr
Ni									Ni-Pt	Ni-Re	Ni-Ru	Ni-Si	Ni-Ta	Ni-Ti	Ni-W	Ni-Zr
Pt										Pt-Re	Pt-Ru	Pt-Si	Pt-Ta	Pt-Ti	Pt-W	Pt-Zr
Re											Re-Ru	Re-Si	Re-Ta	Re-Ti	Re-W	Re-Zr
Ru												Ru-Si	Ru-Ta	Ru-Ti	Ru-W	Ru-Zr
Si													Si-Ta	Si-Ti	Si-W	Si-Zr
Ta														Ta-Ti	Ta-W	Ta-Zr
Ti															Ti-W	Ti-Zr
W																W-Zr

Table 1.4: Current Status of Key Ternary Systems

Al-Co-Ni	Al-Cr-Ni	Al-Co-W	Al-Mo-Ni	Al-Nb-Ni	Al-Ni-Pt	Al-Ni-Re	Al-Ni-Si
Al-Ni-Ta	Al-Ni-Ti	Al-Ni-W	Co-Cr-Mo	Co-Cr-Ni	Co-Cr-Ti	Co-Cr-W	Co-Fe-W
Co-Mo-Ni	Co-Ni-Si	Co-Ni-Ta	Co-Ni-Ti	Co-Ni-W	Cr-Fe-Ni	Cr-Fe-Ti	Cr-Mo-Nb
Cr-Mo-Ni	Cr-Nb-Ni	Cr-Ni-Pt	Cr-Ni-Ru	Cr-Ni-Ta	Cr-Ni-Ti	Cr-Ni-W	Cu-Hf-Ni
Cu-Nb-Ni	Cu-Ni-Si	Cu-Ni-Ta	Cu-Ni-Ti	Cu-Ni-Zr	Fe-Mo-Ni	Fe-Nb-Ni	Fe-Ni-Si
Fe-Ni-W	Mo-Nb-Ni	Mo-Ni-Si	Mo-Ni-Ta	Mo-Ni-W	Nb-Ni-Ti	Ni-Si-Ti	Ni-Ti-W
Al-B-Cr	Al-B-Ni	B-Co-Cr	B-Co-Ni	B-Cr-Fe	B-Cr-Ti	B-Fe-Ni	B-Ni-Ti
B-Ni-W	C-Co-Cr	C-Co-Fe	C-Co-Ni	C-Co-W	C-Cr-Ni	C-Cr-Ti	C-Fe-Ni
C-Fe-W	C-Mo-Ti	C-Mo-W	C-Nb-W	C-Ni-W			

1.6 Database Validation

This database focuses on the nickel-rich corner of multicomponent nickel alloys, and has been extensively tested and validated by a large number of commercial nickel alloys. Table 1.5 lists the alloys and references used for testing the current database. In the table, T_f^{ℓ}, T_f^{s}, and $T_f^{\gamma'}$ represent liquidus, solidus (γ starts to form from liquid), and γ′ solvus (γ′ starts to precipitate in the γ phase matrix) temperatures, respectively. $f^{\gamma'}$ represents the volume fraction of the γ′ phase, and $x(X)\,in\,\gamma$, $x(X)\,in\,\gamma'$ represent the equilibrium compositions of component X in the γ and γ′ phases, respectively. The recommended composition ranges given in Table 1.1 are the ones that have been extensively tested. Users need to be careful when using the database beyond the suggested ranges.

This database can be used to calculate phase equilibria for multi-component alloys, such as the equilibrium between γ and γ′. It can be used to predict phase transformation temperatures, such as liquidus, solidus and γ′ solvus. The fraction of each phase as a function of temperature and 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 calculation results are presented in Figure 1.1 to Figure 1.10.

Figure 1.1 shows comparison between calculated and experimentally measured liquidus and solidus temperatures for nickel-based superalloys, while Figure 1.2 is for that of the solvus temperatures of the γ′ phase. Figure 1.3 shows comparison between calculated and experimentally determined amounts of the γ′ phase. Figure 1.4 to Figure 1.10 are comparisons between the calculated and experimentally measured equilibrium compositions for Al, Co, Cr, Mo, Re, Ti, and W in γ and γ′ phases, respectively. These figures show reasonable agreement between the calculated values using the current nickel database and the experimentally determined ones.

Table 1.5: Experimental Data Used for Testing the Current Nickel Database

Alloy	Experimental Information	References
Udimet-700	$T_f^{\gamma'}$, $f^{\gamma'}$ $vs.T$, $x(Al,Cr,Ti,Mo,W)$ $in\ \gamma'\ vs.T$	[1971Mol]
Ni-14Cr-6.5~12Al-4Ti-1~5Mo	$T_f^{\gamma'}$	[1972Loo]
Ni-4~13Al-6.5~20.5Cr-0.25~4.5Ti-0~6Mo-0~4W	$f^{\gamma'}$ $at\ 850^o C$, $x(Al,Cr,Ti,Mo,W)$ $in\ \gamma\ and\ \gamma'$	[1974Dre]
IN-939	$x(Al,Co,Cr,Ti,Ta,W)$ $in\ \gamma\ and\ \gamma'$	[1983Del]
Udimet-520	$x(Al,Co,Cr,Ti,Mo,W)$ $in\ \gamma\ and\ \gamma'$	[1983Mag]
Udimet-710	$x(Al,Co,Cr,Ti,Mo,W)$ $in\ \gamma\ and\ \gamma'$	[1983Mag]
Udimet-100	$x(Al,Co,Cr,Ti,Mo,W)$ $in\ \gamma\ and\ \gamma'$	[1983Mag]
N-18	$T_f^{\gamma'}$	[1988Duc]
IN-100	$T_f^{\gamma'}$	[1988Duc]
MERL-76	$T_f^{\gamma'}$	[1988Duc]
RENE-95	$T_f^{\gamma'}$	[1988Duc]
ASTROLOY	$T_f^{\gamma'}$	[1988Duc]
Nimonic-105	$x(Al,Co,Cr,Ti,Mo)$ $in\ \gamma\ and\ \gamma'$	[1991Tri]
BJH, BJJ, BJK, BJL, BJM, BJP	T_f^{ℓ}, T_f^{s}, $T_f^{\gamma'}$	[1992Dha]
2D8625, 2D8638, 2D8639, 2D8640	T_f^{ℓ}, T_f^{s}, $T_f^{\gamma'}$	[1992Dha]
MA6000	T_f^{ℓ}, T_f^{s}, $T_f^{\gamma'}$	[1992Dha]
CMSX-2	T_f^{ℓ}, T_f^{s}, $T_f^{\gamma'}$	[1992Dha]
SRR-99	$x(Al,Co,Cr,Ti,Ta,W)$ $in\ \gamma\ and\ \gamma'$	[1992Sch]
Modified IN738LC	$x(Al,Co,Cr,Ta,W,Mo)$ $in\ \gamma\ and\ \gamma'$	[1993Zha]
MC2	$x(Al,Co,Cr,Ta,Ti,W,Mo)$ $in\ \gamma\ and\ \gamma'$	[1994Duv]
Ni-Al-Re-X(X: Cr, Mo, W, Ti, Ta, Nb, Co)	$x(Al,RE,X)$ $in\ \gamma\ and\ \gamma'$	[1994Miy]
Rene N6	T_f^{ℓ}, T_f^{s}, $T_f^{\gamma'}$, $f^{\gamma'}$, $x(Al,Co,Cr,Ta,RE,W,Mo)$ $in\ \gamma\ and\ \gamma'$	[1998Rit] [1999Rit] [2001Cop]

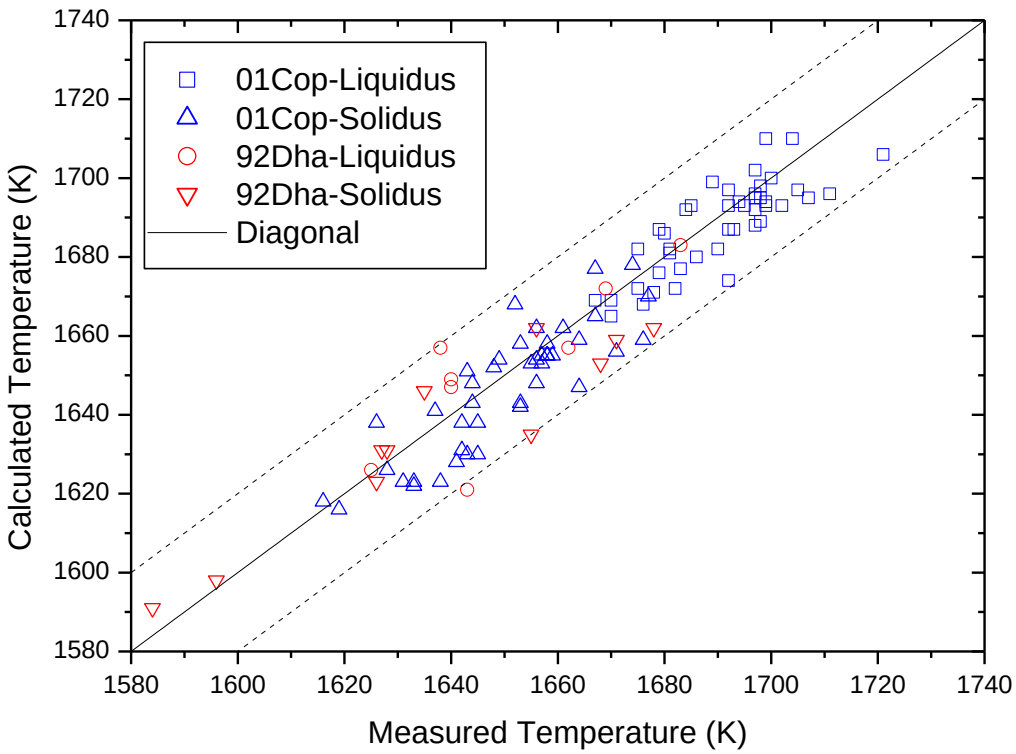

Figure 1.1: Comparison between the calculated and experimentally measured liquidus and solidus temperatures

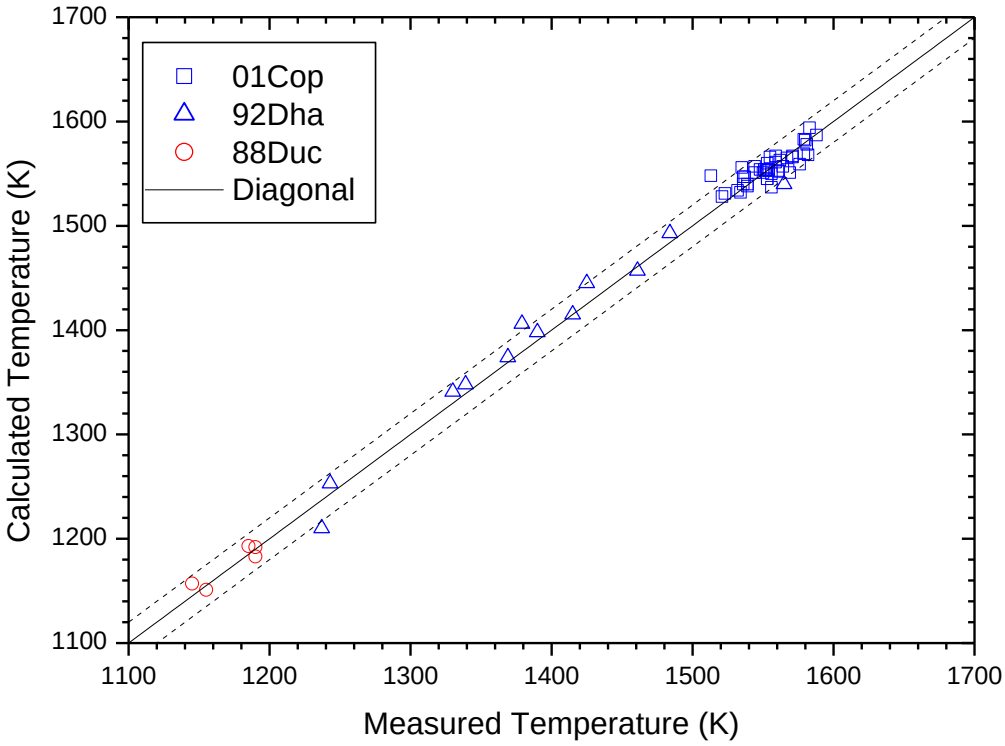

Figure 1.2: Comparison between the calculated and experimentally measured solvus temperatures of the γ′ phase

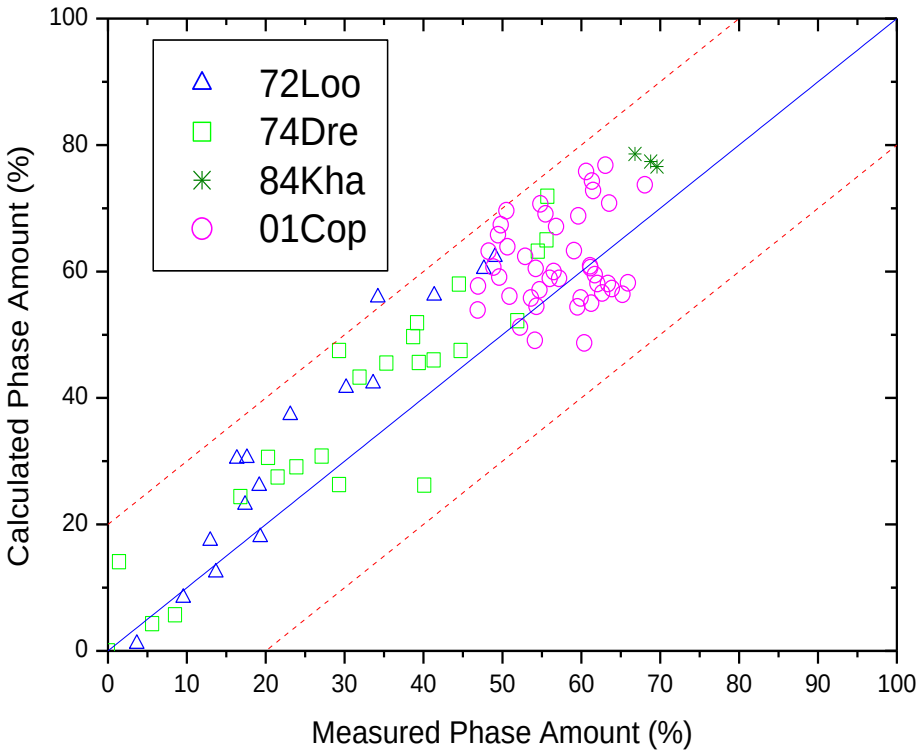

Figure 1.3: Comparison between the calculated and experimentally measured amounts of the γ′ phase

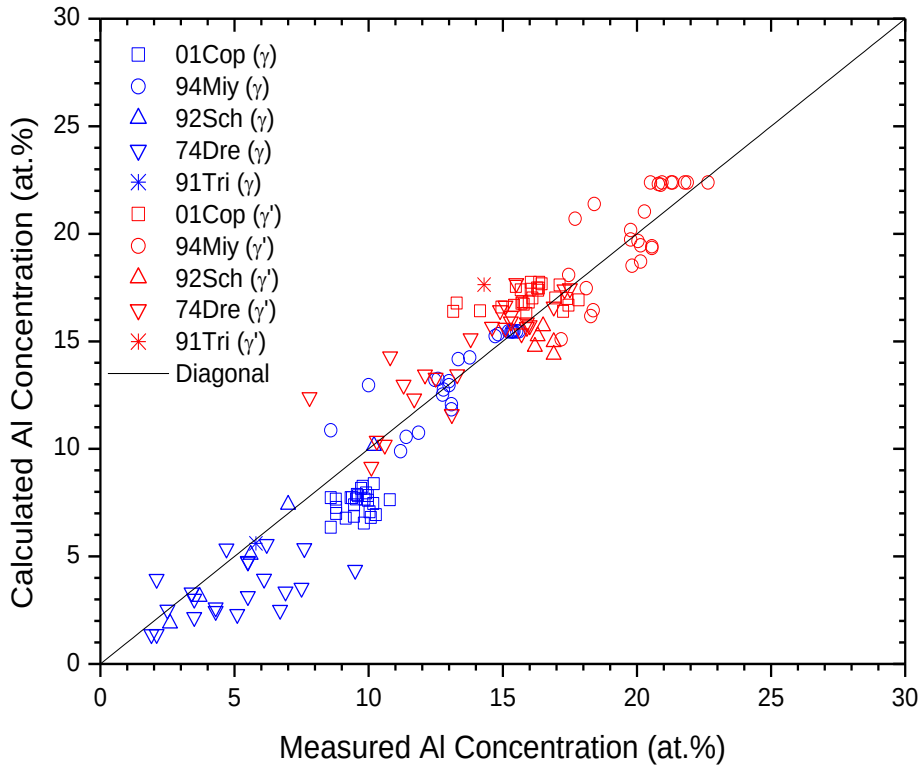

Figure 1.4: Comparison between the calculated and experimentally measured equilibrium compositions of Al in γ and γ′ phase

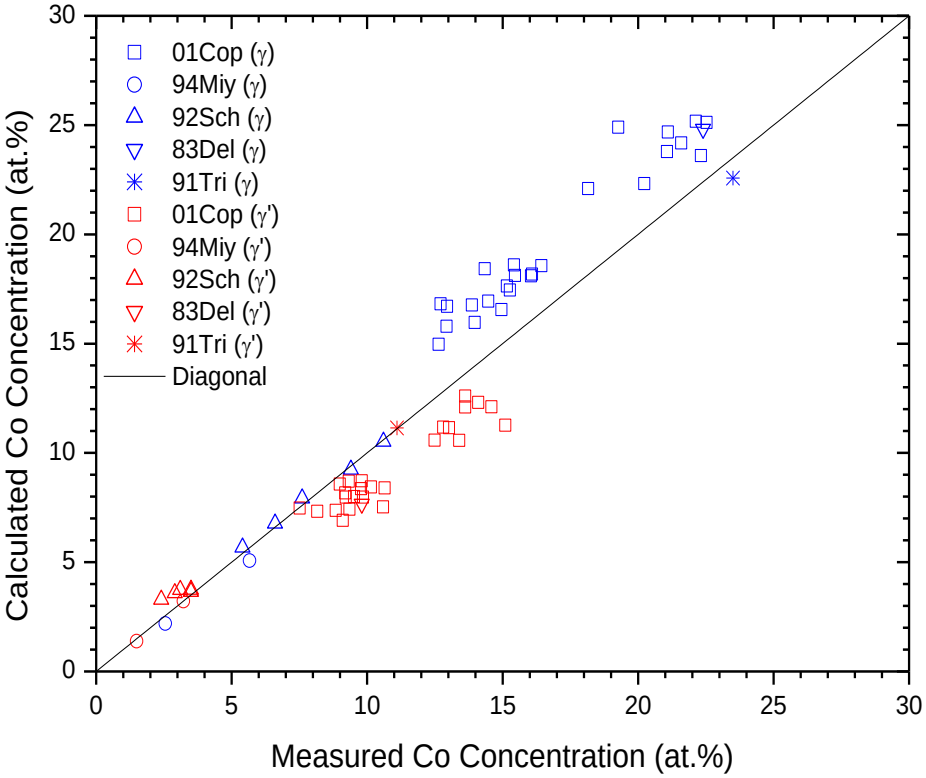

Figure 1.5: Comparison between the calculated and experimentally measured equilibrium compositions of Co in γ and γ′ phases

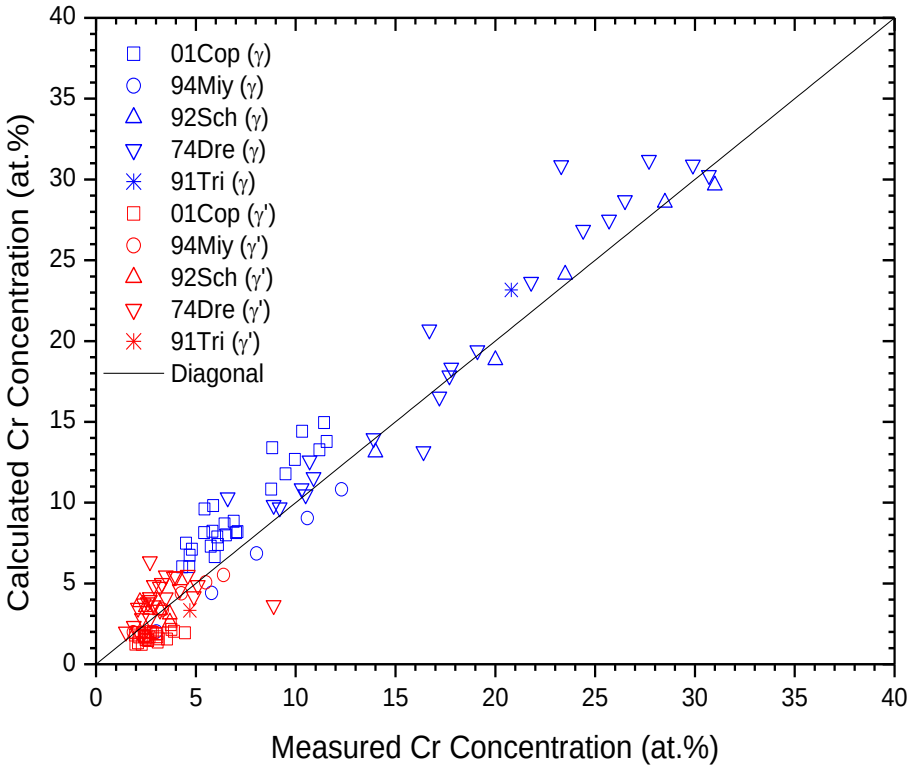

Figure 1.6: Comparison between the calculated and experimentally measured equilibrium compositions of Cr in γ and γ′ phases

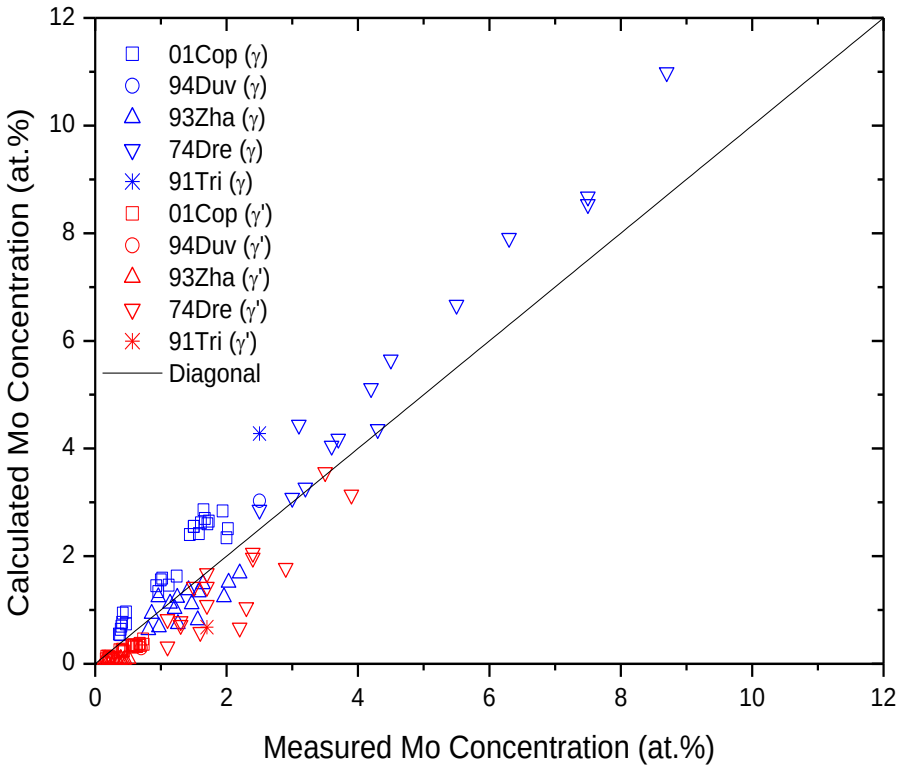

Figure 1.7: Comparison between the calculated and experimentally measured equilibrium compositions of Mo in γ and γ′ phases

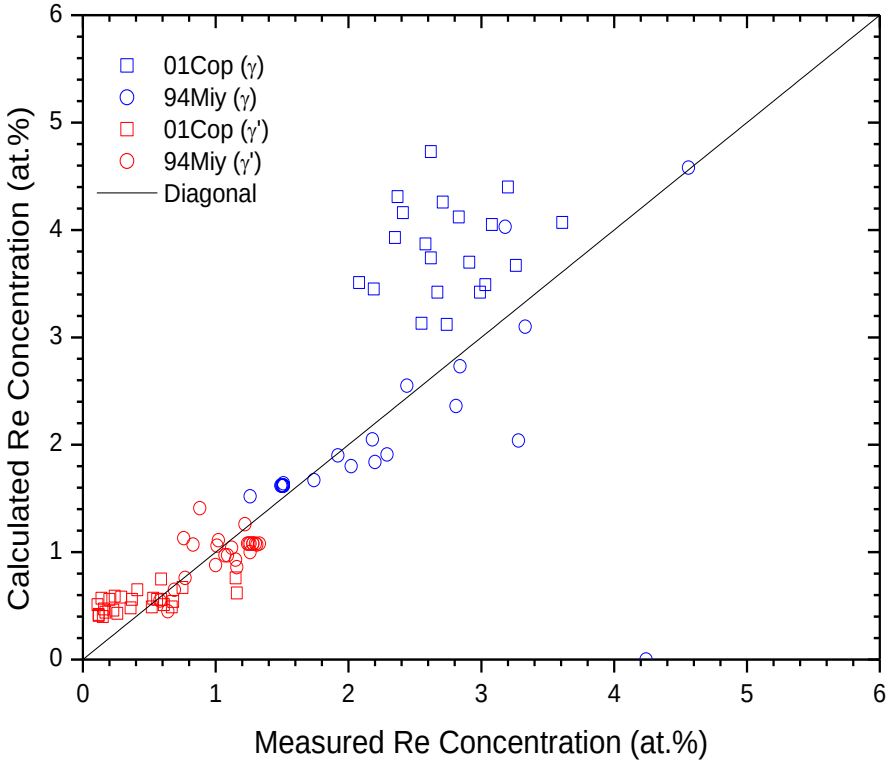

Figure 1.8: Comparison between the calculated and experimentally measured equilibrium compositions of Re in γ and γ′ phases

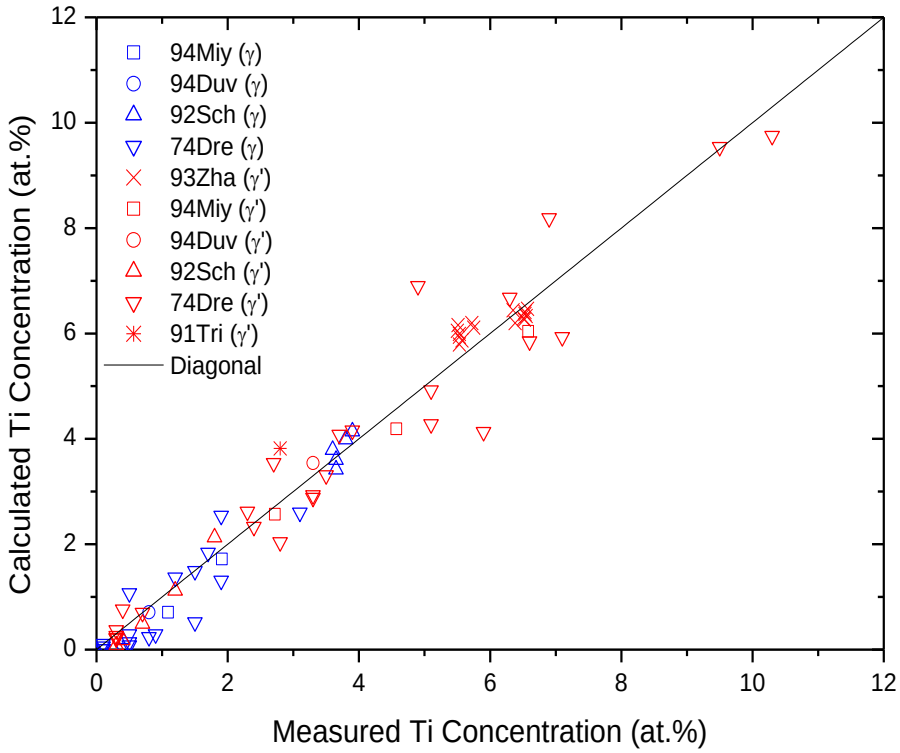

Figure 1.9: Comparison between the calculated and experimentally measured equilibrium compositions of Ti in γ and γ′ phases

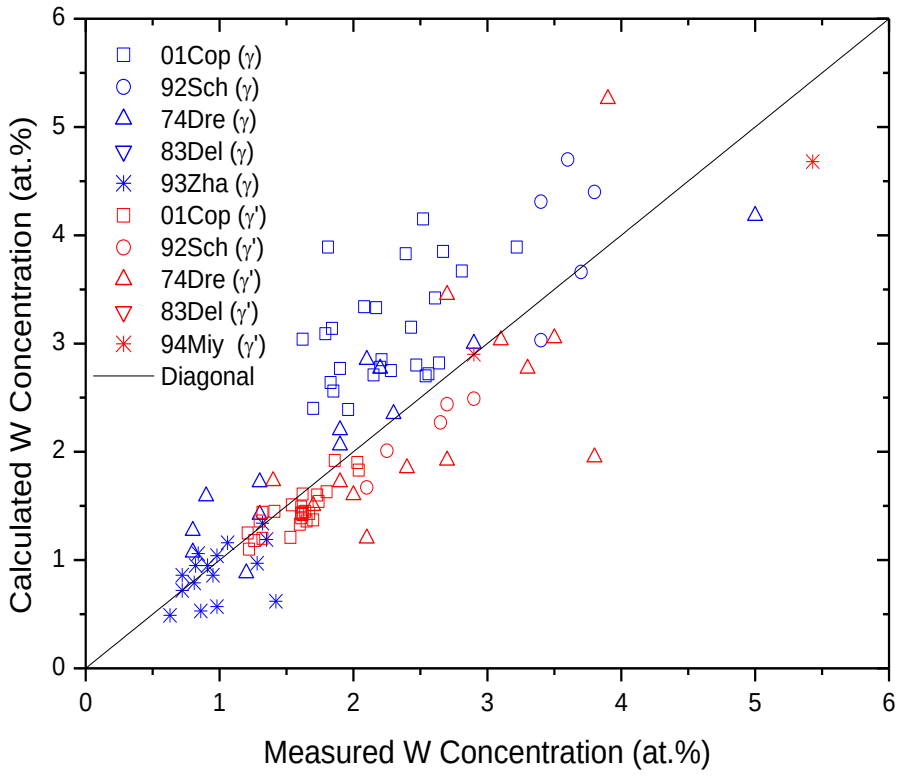

Figure 1.10: Comparison between the calculated and experimentally measured equilibrium compositions of W in γ and γ′ phases

1.7 References

[1971Mol] E. H. van der Molen, J. M. Oblak and O. H. Kriege, Metal. Trans. 2 (1971) 1627-1633.

[1972Loo] W. T. Loomis, J. W. Freeman and D. L. Sponseller, Metal. Trans. 3 (1972) 989-1000.

[1974Dre] R. L. Dreshfield and J. F. Wallace, Metal. Trans. 5 (1974) 71-78.

[1983Del] K. M. Delargy and G. D. W. Smith, Metal. Trans. 14A (1983) 1771-1783.

[1983Mag] M. Magrini, B. Badan and E. Ramous, Z. Metallkde. 74 (1983) 314-316.

[1988Duc] C. Ducrocq, A. Lasalmonie and Y. Honnorat, in: S. Reichman, D. N. Duhl, G. Maurer, S. Antolovich and C. Lund (Eds.), Superalloys, The Metallurgical Society, 1988, pp. 63-72.

[1991Tri] K. Trinckauf and E. Nembach, Acta Metall. Mater. 39(12) (1991) 3057-3061.

[1992Dha] S.-R. Dharwadkar, K. Hilpert, F. Schubert and V. Venugopal, Z. Metallkde. 83 (1992) 744-749.

[1992Sch] R. Schmidt and M. Feller-Kniepmeier, Scripta Metal. Mater. 26 (1992) 1919-1924.

[1993Zha] J. S. Zhang, Z.Q. Hu, Y. Murata, M. Morinaga and N. Yukawa, Metal. Trans. 24A (1993) 2443-2450.

[1994Duv] S. Duval, S. Chambreland, P. Caron and D. Blavette, Acta Metall. Mater. 42(1) (1994) 185-194.

[1994Miy] S. Miyazaki, Y. Murata and M. Morinaga, Iron and Steel (Japan) 80(2) (1994) 78-83.

[1998Rit] F. J. Ritzert, D. Arenas, D. Keller and V. Vasudevan, NASA/TM 1998-206622.

[1999Rit] F. J. Ritzert, D. Keller and V. Vasudevan, NASA/TM 1999-209277.

[2001Cop] E. H. Copland, N. S. Jacobson and F. J. Ritzert, NASA/TM 2001-210897.