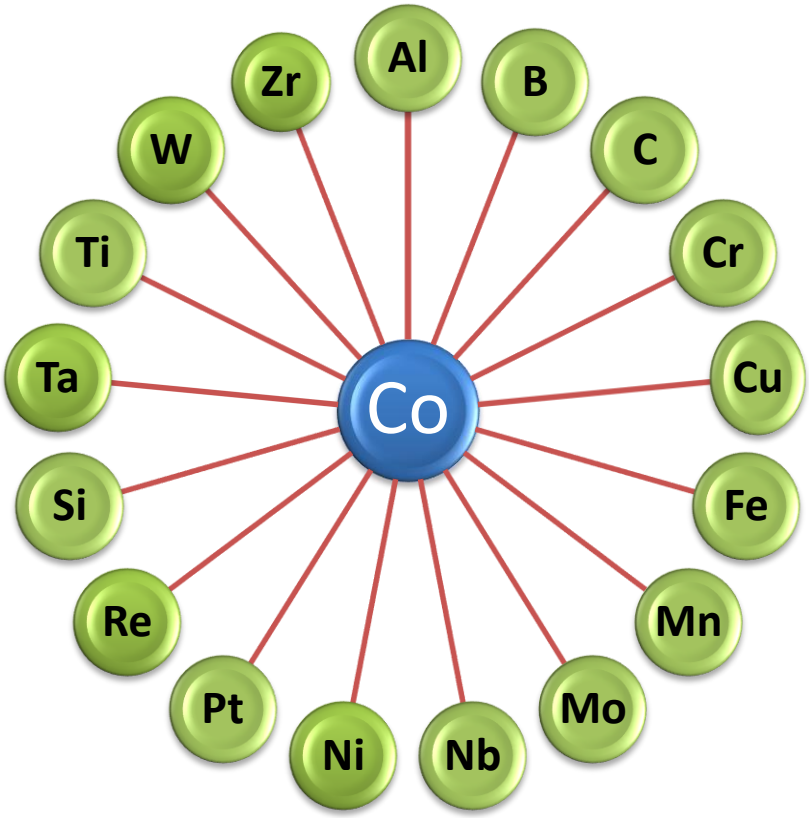
1. PanCobalt

Thermodynamic Database for Cobalt-Based Superalloys



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1.1 Components

A total of 18 components are included in the database as listed here:

Al-B-C-**Co**-Cr-Cu-Fe-Mn-Mo-Nb-Ni-Pt-Re-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 1.3 and Table 1.4.

Table 1.1: Suggested composition range

Element	Composition range (wt%)
Co	50-100
Al	0-50
B,C,Cu,Mn,Pt,Si	0-0.5
Cr	0-30
Mo	0-20
Nb	0-10
Ni	0-50
Fe	0-20
Re	0-20
Ta	0-20
Ti	0-10
W	0-20
Zr	0-10

1.3 Phases

A total of 303 phases are included in the current database. The names and thermodynamic models of major phases are given in Table 1.2. Information on all the other phases may 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,Cu,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,W) (Co,Cr,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,W,Zr,Va)
Bcc	(1)(3)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,W,Zr) (B,C,Va)
Chi	(24)(10)(24)	(Cr,Fe,Mo,Ni,Re)(Cr,Mo,Nb,Re,Ta,W) (Cr,Fe,Nb,Ni,Re,Ta,W)
Fcc	(1)(1)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,W,Zr) (B,C,Va)
Hcp	(1)(0.5)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,W,Zr) (B,C,Va)
L12	(0.75)(0.25) (1)	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,W,Zr) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,W,Zr)(Va)
Laves_C14	(2)(1)	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Re,Ta,Ti,Zr) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Ta,Ti,W,Zr)
Laves_C15	(2)(1)	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Ta,Ti,W,Zr) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ta,Ti,W,Zr)
Laves_C36	(2)(1)	(Al,Co,Cr,Fe,Mn,Ni,Ta,Ti,Zr) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ta,Ti,Zr)
Liquid	(1)	(Al,B,C,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,W, Zr)
Mu	(7)(2)(4)	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Ta,W) (Mo,Nb,Ta,Ti,W) (Co,Cr,Fe,Mo,Nb,Ni,Ta,Ti,W)
Sigma	(8)(4)(18)	(Al,Co,Cr,Fe,Mn,Ni,Pt,Re,Ta,W) (Cr,Fe,Mo,Nb,Re,Ta,Ti,W) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Pt,Re,Ta,Ti,W)

1.4 Key Elements and Subsystems

The current modeling status for the constituent binaries and ternaries are given in Table 1.3 and Table 1.4. The color represents the following meaning:

: Full description

: Full description for major phases

: Partial description for major phases

Table 1.3: Modeling status of key constituent binary systems

	B	C	Co	Cr	Cu	Fe	Mn	Mo	Nb	Ni	Pt	Re	Si	Ta	Ti	W	Zr
Al	Al-B	Al-C	Al-Co	Al-Cr	Al-Cu	Al-Fe	Al-Mn	Al-Mo	Al-Nb	Al-Ni	Al-Pt	Al-Re	Al-Si	Al-Ta	Al-Ti	Al-W	Al-Zr
B		B-C	B-Co	B-Cr	B-Cu	B-Fe	B-Mn	B-Mo	B-Nb	B-Ni	B-Pt	B-Re	B-Si	B-Ta	B-Ti	B-W	B-Zr
C			C-Co	C-Cr	C-Cu	C-Fe	C-Mn	C-Mo	C-Nb	C-Ni	C-Pt	C-Re	C-Si	C-Ta	C-Ti	C-W	C-Zr
Co				Co-Cr	Co-Cu	Co-Fe	Co-Mn	Co-Mo	Co-Nb	Co-Ni	Co-Pt	Co-Re	Co-Si	Co-Ta	Co-Ti	Co-W	Co-Zr
Cr					Cr-Cu	Cr-Fe	Cr-Mn	Cr-Mo	Cr-Nb	Cr-Ni	Cr-Pt	Cr-Re	Cr-Si	Cr-Ta	Cr-Ti	Cr-W	Cr-Zr
Cu						Cu-Fe	Cu-Mn	Cu-Mo	Cu-Nb	Cu-Ni	Cu-Pt	Cu-Re	Cu-Si	Cu-Ta	Cu-Ti	Cu-W	Cu-Zr
Fe							Fe-Mn	Fe-Mo	Fe-Nb	Fe-Ni	Fe-Pt	Fe-Re	Fe-Si	Fe-Ta	Fe-Ti	Fe-W	Fe-Zr
Mn								Mn-Mo	Mn-Nb	Mn-Ni	Mn-Pt	Mn-Re	Mn-Si	Mn-Ta	Mn-Ti	Mn-W	Mn-Zr
Mo									Mo-Nb	Mo-Ni	Mo-Pt	Mo-Re	Mo-Si	Mo-Ta	Mo-Ti	Mo-W	Mo-Zr
Nb										Nb-Ni	Nb-Pt	Nb-Re	Nb-Si	Nb-Ta	Nb-Ti	Nb-W	Nb-Zr
Ni											Ni-Pt	Ni-Re	Ni-Si	Ni-Ta	Ni-Ti	Ni-W	Ni-Zr
Pt												Pt-Re	Pt-Si	Pt-Ta	Pt-Ti	Pt-W	Pr-Zr
Re													Re-Si	Re-Ta	Re-Ti	Re-W	Re-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: Modeling status of key constituent ternary systems

Al-Co-Cr	Al-Co-Mn	Al-Co-Nb	Al-Co-Ni	Al-Co-W	Al-Cr-Ni	Al-Cr-Ti	Al-Fe-Mo
Al-Fe-Ni	Al-Mn-Ni	Al-Mn-Si	Al-Mo-Ni	Al-Mo-Ti	Al-Nb-Ti	Al-Ni-Si	Al-Ni-Ti
Al-Ni-W	Al-Ta-Ti	Co-Cr-Fe	Co-Cr-Mo	Co-Cr-Nb	Co-Cr-Ni	Co-Cr-Ti	Co-Cr-W
Co-Cu-Fe	Co-Mn-Ni	Co-Mo-W	Co-Ni-W	Cr-Mn-Ni	Cr-Nb-Ni	Cr-Ni-Si	Cr-Ni-W
Fe-Nb-Ni	Fe-Ni-Ti	Mn-Ni-Si	Mn-Nb-Ta	Re-Ta-W	C-Al-Co		
C-Al-Fe	C-Al-Ni	C-Co-Cr	C-Co-Fe	C-Co-Mo	C-Co-Nb	C-Co-Ta	C-Co-Ti
C-Cr-Fe	C-Cr-Mo	C-Fe-Mn	C-Mo-Ti	Al-Co-Ta	Al-Co-Ti	Al-Fe-Ta	Al-Nb-Ni
Al-Ni-Ta	Co-Cr-Ta	Co-Fe-Mn	Co-Fe-Mo	Co-Fe-Ni	Co-Fe-Ta	Co-Fe-W	Co-Mo-Ni
Co-Mo-Ta	Co-Mo-Ti	Co-Nb-Ti	Co-Ni-Ta	Co-Ni-Ti	Co-Ta-Ti	Cr-Fe-Mn	Cr-Fe-Mo
Cr-Fe-Ni	Cr-Mo-Ni	Cr-Mo-Ta	Cr-Ni-Ti	Cr-Ta-W	Fe-Mn-Nb	Fe-Mn-Ti	Fe-Mo-Ti
Mn-Nb-Si	Mn-Ni-Ta	Mn-Ni-Ti	Nb-Si-W	Ni-Re-W			
C-Al-Co	C-Al-Ti	C-Co-Mn	C-Co-Ni	C-Co-W	C-Cr-Ni	C-Cr-W	C-Fe-Ni
C-Fe-W	C-Mo-Ti	C-Mo-W	C-Ni-W	C-Si-Ti			

1.5 Database Validation

The current thermodynamic database for cobalt alloys has been extensively tested and validated using the published experimental data [2008Ish, 2008Shi, 2010Bau, 2010Pol, 2012Bau, 2015Mak, 2015Mak2]. Figure 1.1 and Figure 1.2 show two calculated isopleth in the Co-Al-Ni-W quaternary system compared with the experimental data [2008Ish, 2008Shi]. The isopleth in Figure 1.1 is a vertical section at 10 at% of Al and 7.5 at% of W and that in Figure 1.2 is at 10 at.% of Al and 10 at.% of W. In both figures, the calculated phase boundaries are in good agreement with the experimental data. Makineni et al. [2015Mak, 2015Mak2] discovered a new class of γ/γ' Co-based superalloy that is free of tungsten, with the composition of Co-10Al-5Mo-2Nb (in at.%). The solvus temperature can be further enhanced by addition of Ni to form Co-xNi-10Al-5Mo-2Nb, where x can be from 0 to 30 at.%. The comparison between the calculated and measured γ' solvus is shown in Figure 1.3. Figure 1.4 and Figure 1.5 show two calculated isothermal sections with fixed Ni content at 60 at% for the Co-Ni-Al-Cr quaternary system at 1100°C and 1000°C, respectively. The calculated results agree well with the experimental observations from annealed alloy samples [2006Bur]. Figure 1.6 shows the comparison between the calculated liquidus, solidus and γ′ solvus temperatures and the experimentally measured ones [2010Bau, 2010Pol, 2012Bau].

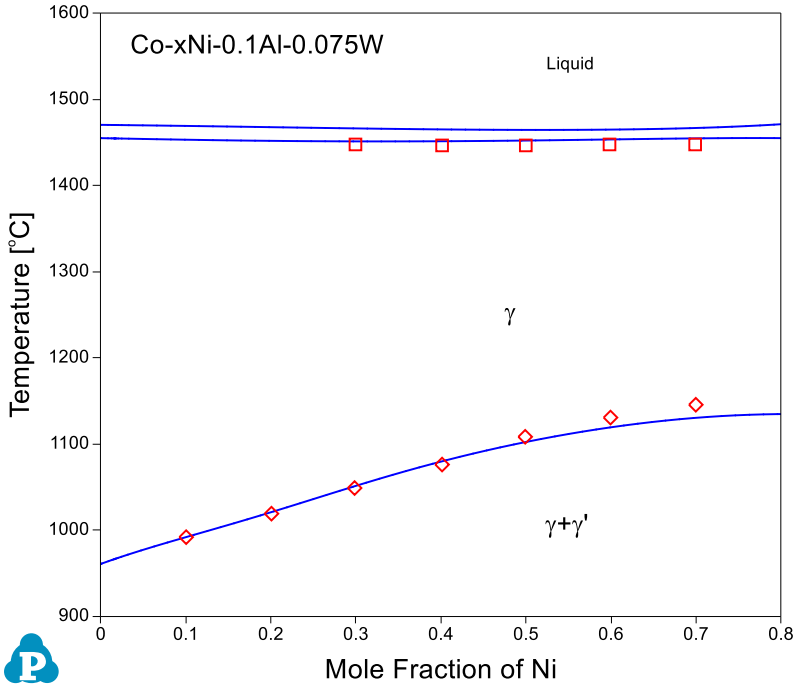

Figure 1.1: Comparison between calculated and measured γ′ solvus and solidus temperatures of Co-xNi-10Al-7.5W alloys

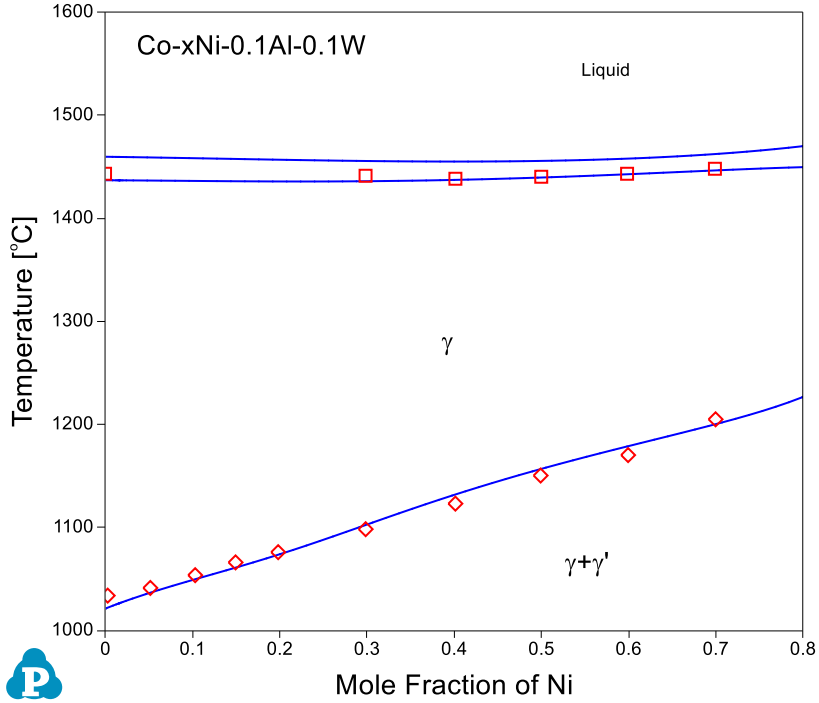

Figure 1.2: Comparison between calculated and measured γ′ solvus and solidus temperatures of Co-xNi-10Al-10W alloys

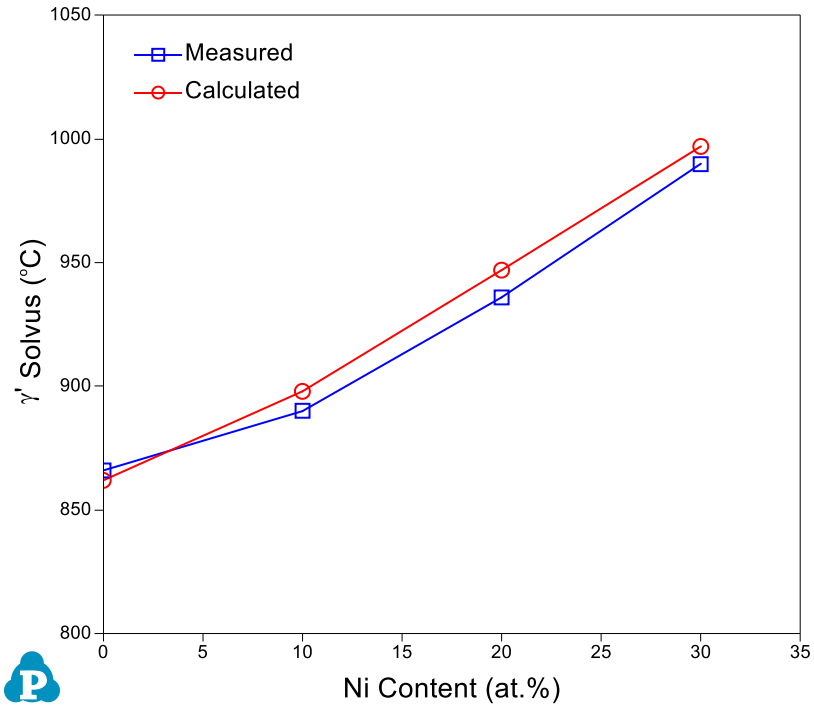

Figure 1.3: Comparison between the calculated and measured γ' solvus for Co-xNi-10Al-5Mo-2Nb alloys

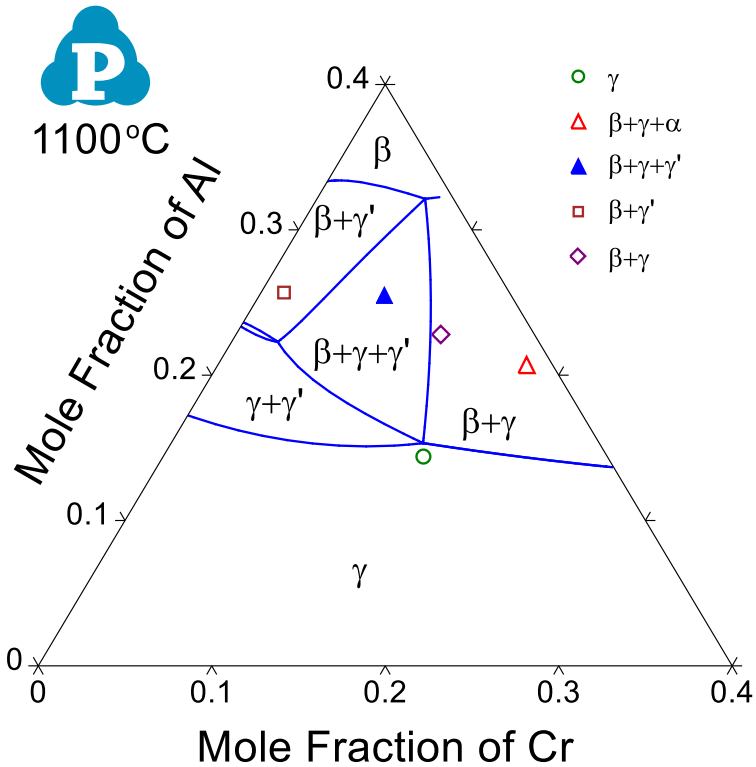

Figure 1.4: Calculated 1100 °C isothermal section of Co-Ni-Al-Cr system with fixed Ni content at 60 at.% compared with experimental observations

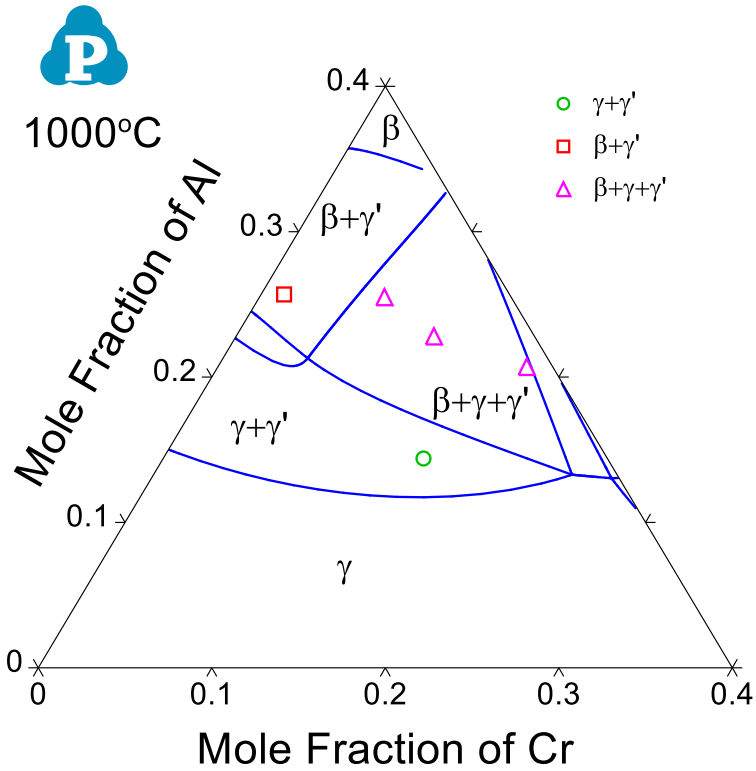

Figure 1.5: Calculated 1000 °C isothermal section of Co-Ni-Al-Cr system with fixed Ni content at 60 at.% compared with experimental observations

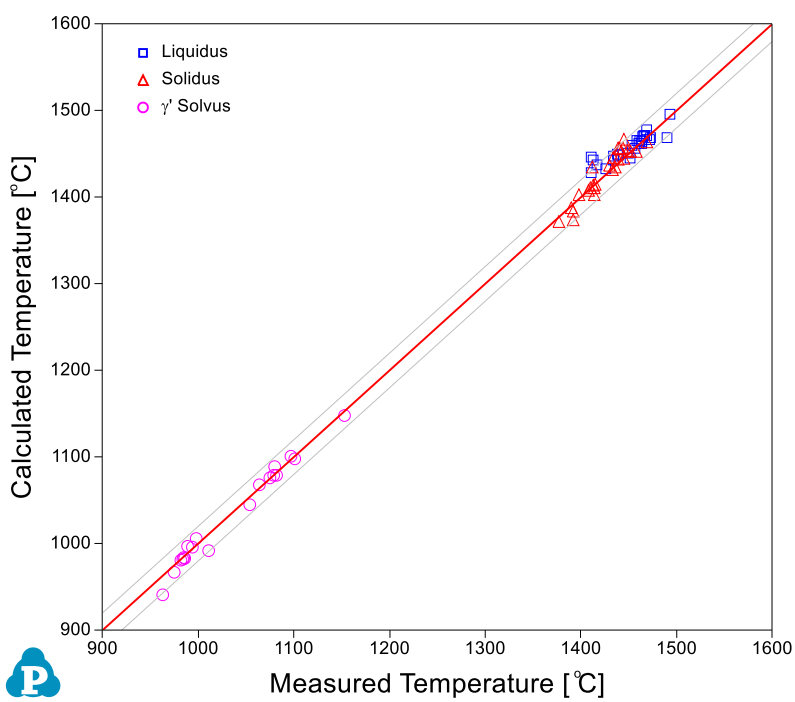

Figure 1.6: Comparison between calculated results and experimental data for Liquidus, solidus and γ′ solvus temperatures.

1.6 Referneces

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