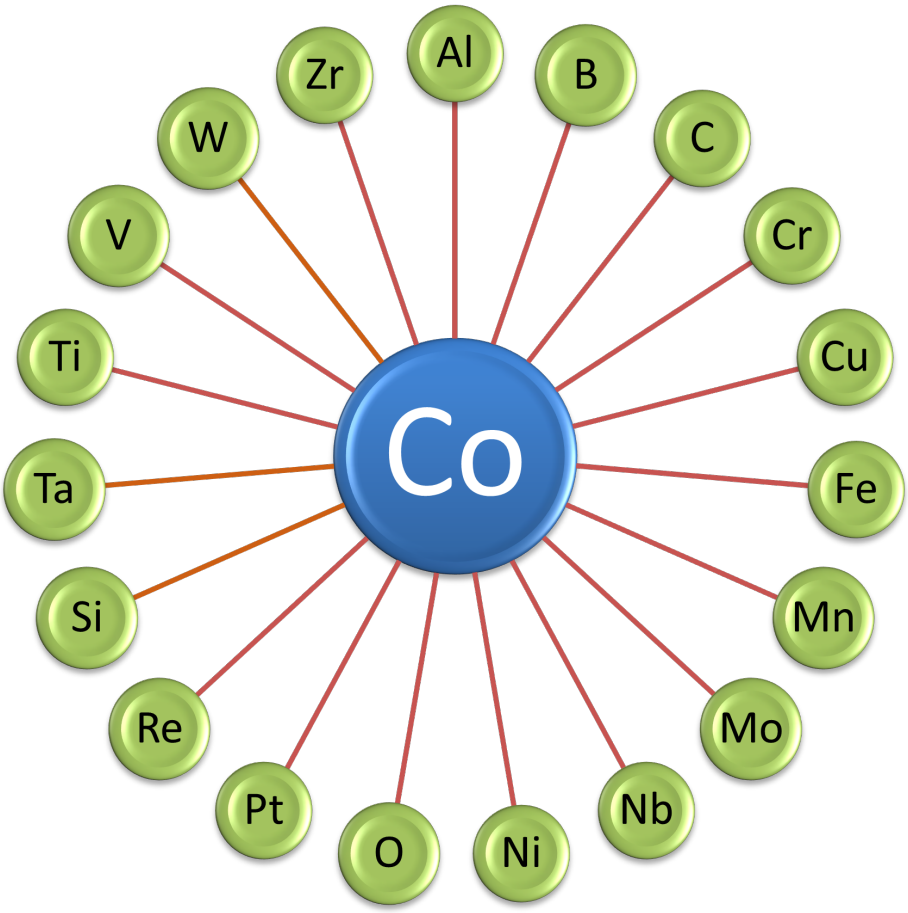
Pandat 2025

Database Manual

CompuTherm LLC

PanCobalt

Database for multi-component Cobalt-based Superalloys



PANDAT™
SOFTWARE

Contents

1 Thermodynamic Database

1.1 Components (20)

A total of **20** components are included in the database as listed here:

Al-B-C-**Co**-Cr-Cu-Fe-Mn-Mo-Nb-Ni-O-Pt-Re-Si-Ta-Ti-V-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 Section 1.4 .

Table 1.1: Suggested composition range

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

1.3 Phases

Total of **379** phases are included in the current database. The names and thermodynamic models of some phases are given in Table 1.2. Information on all the other phases is listed in PanCo2025:List of All Phases. Users can also view it through TDB viewer of Pandat .

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,V,W,Zr) (B,C,O,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,V,W,Zr) (B,C,Va)
Hcp	(1)(0.5)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,V,W,Zr) (B,C,O,Va)
L12	(0.75)(0.25) (1)	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,V,W,Zr) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,V,W,Zr)(Va)
Laves_C14	(2)(1)	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Re,Ta,Ti,V,Zr) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Ta,Ti,V,W,Zr)
Laves_C15	(2)(1)	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Ta,Ti,V,W,Zr) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ta,Ti,V,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,O,Pt,Re,Si,Ta,Ti,V,W,Zr, Al2O3,B2O3,CoO,Co2O3,Cr2/3O,CuO,Cu2O,Cu2O3,FeO, FeO3/2,MnO,MnO3/2,MoO2,MoO3,NbO,NbO2,NbO5/2,NiO, SiO2,Ta2O5,TiO,TiO3/2,TiO2,VO,VO2,VO3/2,VO5/2,WO2, WO3,Zr1/2O)
Mu	(7)(2)(4)	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Ta,W)

Name	Lattice Size	Constituent
		(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,V,W) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Pt,Re,Ta,Ti,V,W)

1.4 Assessed Subsystems

A total of **277** subsystems, including 187 binary and 90 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 (187)

Al-B(10)	Al-C(10)	Al-Co(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-Pt(10)	Al-Re(10)	Al-Si(10)
Al-Ta(10)	Al-Ti(10)	Al-V(10)	Al-W(10)	Al-Zr(10)	B-C(10)	B-Co(10)
B-Cr(10)	B-Cu(10)	B-Fe(10)	B-Mn(10)	B-Mo(10)	B-Nb(10)	B-Ni(10)
B-O(10)	B-Pt(10)	B-Re(10)	B-Si(10)	B-Ta(10)	B-Ti(10)	B-V(10)
B-W(10)	B-Zr(10)	C-Co(10)	C-Cr(10)	C-Cu(10)	C-Fe(10)	C-Mn(10)
C-Mo(10)	C-Nb(10)	C-Ni(10)	C-O(10)	C-Pt(10)	C-Re(10)	C-Si(10)
C-Ta(10)	C-Ti(10)	C-V(10)	C-W(10)	C-Zr(10)	Co-Cr(10)	Co-Cu(10)
Co-Fe(10)	Co-Mn(10)	Co-Mo(10)	Co-Nb(10)	Co-Ni(10)	Co-O(10)	Co-Pt(10)
Co-Re(10)	Co-Si(10)	Co-Ta(10)	Co-Ti(10)	Co-V(10)	Co-W(10)	Co-Zr(10)
Cr-Cu(10)	Cr-Fe(10)	Cr-Mn(10)	Cr-Mo(10)	Cr-Nb(10)	Cr-Ni(10)	Cr-O(10)
Cr-Pt(10)	Cr-Re(10)	Cr-Si(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-Pt(10)	Cu-Re(10)	Cu-Si(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-Pt(10)
Fe-Re(10)	Fe-Si(10)	Fe-Ta(10)	Fe-Ti(10)	Fe-V(10)	Fe-W(10)	Fe-Zr(10)
Mn-Mo(10)	Mn-Nb(10)	Mn-Ni(10)	Mn-O(10)	Mn-Pt(10)	Mn-Re(8)	Mn-Si(10)
Mn-Ta(10)	Mn-Ti(10)	Mn-V(10)	Mn-W(6)	Mn-Zr(10)	Mo-Nb(10)	Mo-Ni(10)
Mo-O(10)	Mo-Pt(10)	Mo-Re(10)	Mo-Si(10)	Mo-Ta(10)	Mo-Ti(10)	Mo-V(10)
Mo-W(10)	Mo-Zr(10)	Nb-Ni(10)	Nb-O(10)	Nb-Pt(10)	Nb-Re(10)	Nb-Si(10)
Nb-Ta(10)	Nb-Ti(10)	Nb-V(10)	Nb-W(10)	Nb-Zr(10)	Ni-O(10)	Ni-Pt(10)
Ni-Re(10)	Ni-Si(10)	Ni-Ta(10)	Ni-Ti(10)	Ni-V(10)	Ni-W(10)	Ni-Zr(10)
O-Pt(5)	O-Re(5)	O-Si(10)	O-Ta(10)	O-Ti(10)	O-V(10)	O-W(10)
O-Zr(10)	Pt-Re(10)	Pt-Si(10)	Pt-Ta(10)	Pt-Ti(10)	Pt-W(10)	Pt-Zr(10)
Re-Si(10)	Re-Ta(10)	Re-Ti(10)	Re-W(10)	Re-Zr(10)	Si-Ta(10)	Si-Ti(10)
Si-V(10)	Si-W(10)	Si-Zr(10)	Ta-Ti(10)	Ta-V(10)	Ta-W(10)	Ta-Zr(10)
Ti-V(10)	Ti-W(10)	Ti-Zr(10)	V-Zr(10)	W-Zr(10)		

Ternary Systems (90)

Al-C-Co(10)	Al-C-Fe(6)	Al-C-Ni(6)	Al-Co-Cr(8)	Al-Co-Mn(8)	Al-Co-Nb(10)
Al-Co-Ni(10)	Al-Co-Ta(5)	Al-Co-Ti(5)	Al-Co-W(10)	Al-Cr-Ni(8)	Al-Cr-Ti(8)
Al-Fe-Mo(10)	Al-Fe-Ni(8)	Al-Fe-Ta(5)	Al-Mn-Ni(8)	Al-Mn-Si(10)	Al-Mo-Ni(8)
Al-Mo-Ti(10)	Al-Nb-Ni(5)	Al-Nb-Ti(10)	Al-Ni-Si(10)	Al-Ni-Ta(7)	Al-Ni-Ti(8)
Al-Ni-W(10)	Al-Ta-Ti(10)	C-Co-Cr(8)	C-Co-Fe(8)	C-Co-Mo(6)	C-Co-Nb(6)
C-Co-Ta(6)	C-Co-Ti(6)	C-Cr-Fe(8)	C-Cr-Mo(6)	C-Fe-Mn(8)	C-Mo-Ti(8)
Co-Cr-Fe(8)	Co-Cr-Mo(8)	Co-Cr-Nb(8)	Co-Cr-Ni(8)	Co-Cr-Ta(2)	Co-Cr-Ti(10)
Co-Cr-W(8)	Co-Cu-Fe(8)	Co-Fe-Mn(5)	Co-Fe-Mo(5)	Co-Fe-Ni(5)	Co-Fe-Ta(6)
Co-Fe-W(6)	Co-Mn-Ni(8)	Co-Mo-Ni(5)	Co-Mo-Ta(5)	Co-Mo-Ti(5)	Co-Mo-W(8)
Co-Nb-Ti(5)	Co-Ni-Si(5)	Co-Ni-Ta(6)	Co-Ni-Ti(5)	Co-Ni-W(10)	Co-Ta-Ti(7)
Cr-Fe-Mn(7)	Cr-Fe-Mo(6)	Cr-Fe-Ni(7)	Cr-Mn-Ni(10)	Cr-Mo-Ni(5)	Cr-Mo-Ta(5)
Cr-Nb-Ni(10)	Cr-Ni-Si(10)	Cr-Ni-Ti(5)	Cr-Ni-W(10)	Cr-Ta-W(6)	Fe-Mn-Nb(7)
Fe-Mn-Ti(6)	Fe-Mo-Ti(5)	Fe-Nb-Ni(8)	Fe-Ni-Si(8)	Fe-Ni-Ti(10)	Mn-Nb-Si(5)
Mn-Nb-Ta(10)	Mn-Ni-Si(10)	Mn-Ni-Ta(5)	Mn-Ni-W(5)	Mo-Ni-Ta(6)	Mo-Ni-Ti(6)

Mo-Ta-W(6) Nb-Ni-Ti(7) Nb-Si-W(5) Ni-Re-W(5) Ni-Si-Ti(10) Re-Ta-W(10)

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].

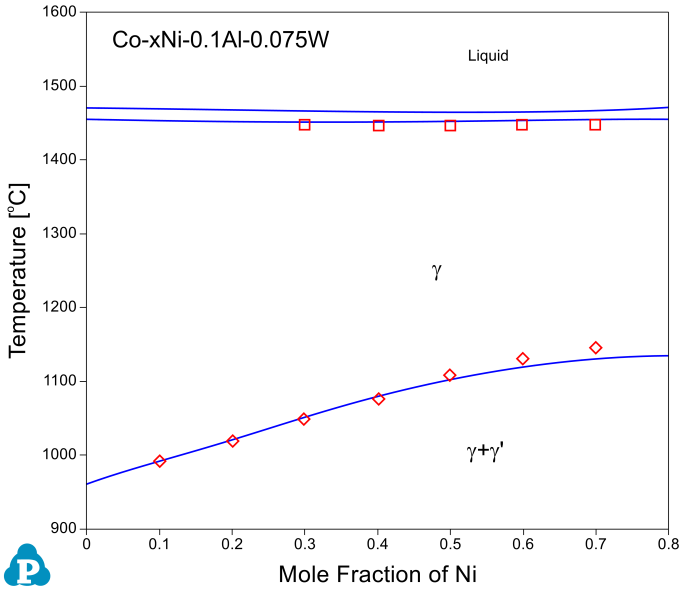


Figure 1.1: Comparison between calculated and measured γ' solvus and solidus temperatures of Co-xNi-10Al-7.5W alloys

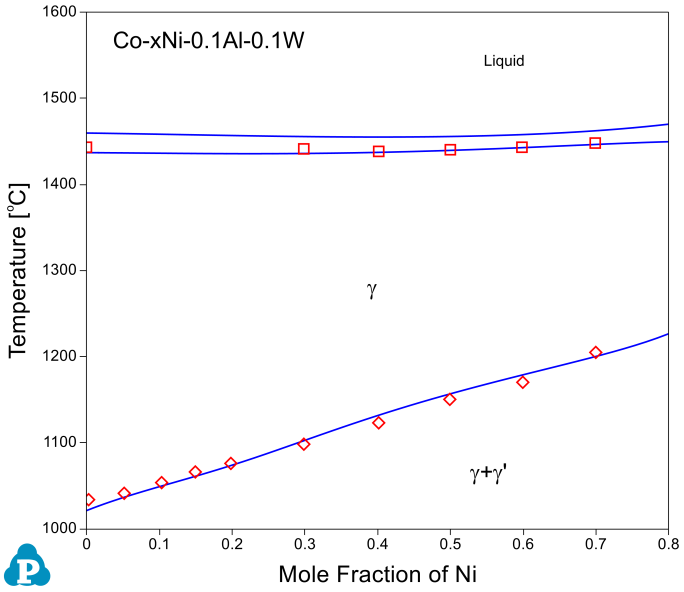


Figure 1.2: Comparison between calculated and measured γ' solvus and solidus temperatures of Co-xNi-10Al-10W alloy

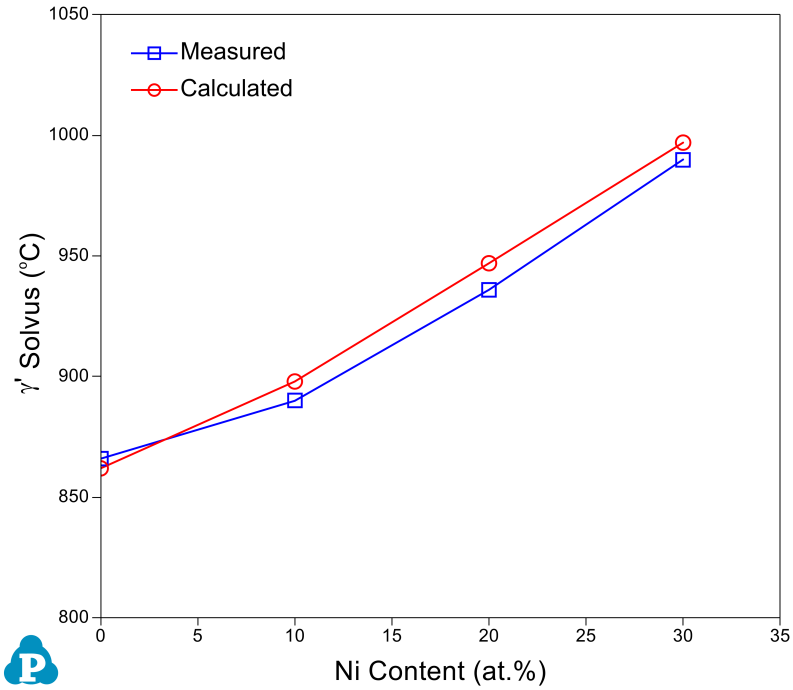


Figure 1.3: Comparison between the calculated and measured γ' solvus for Co-xNi-10Al-5Mo-2Nb alloys

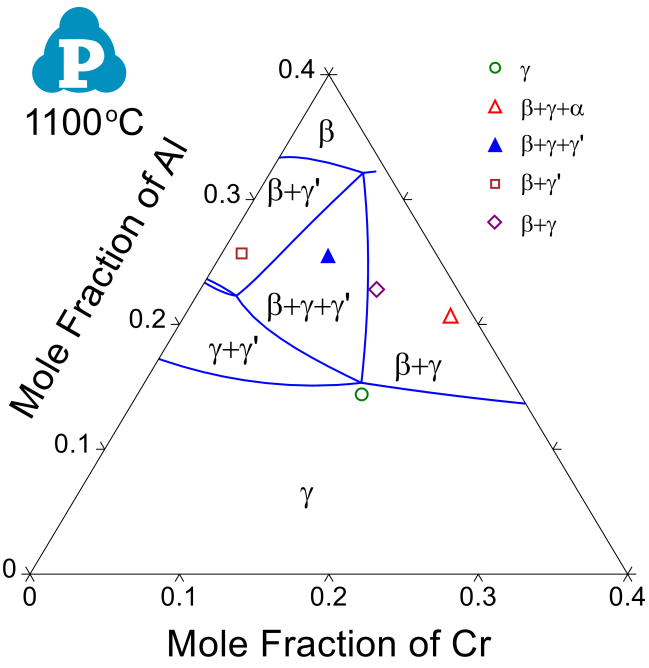


Figure 1.4: Calculated 1100 °C isothermal section of Co-Ni-Al-Cr system with fixed Ni content at 60 at.% compared with experimental observations

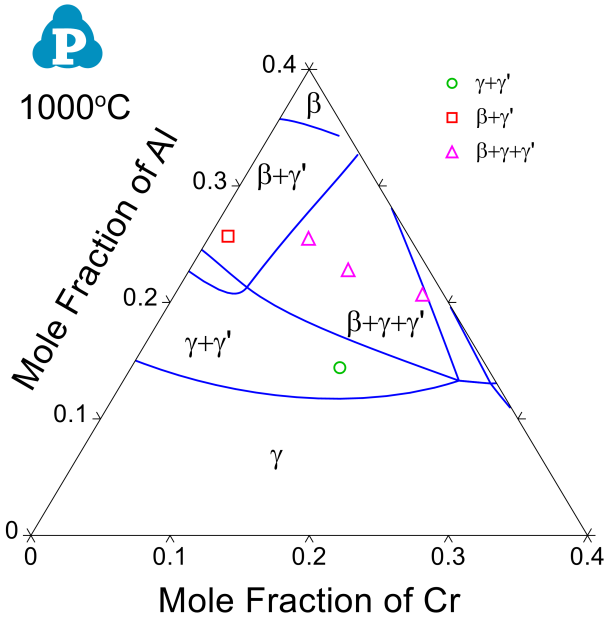


Figure 1.5: Calculated 1000 °C isothermal section of Co-Ni-Al-Cr system with fixed Ni content at 60 at.% compared with experimental observations

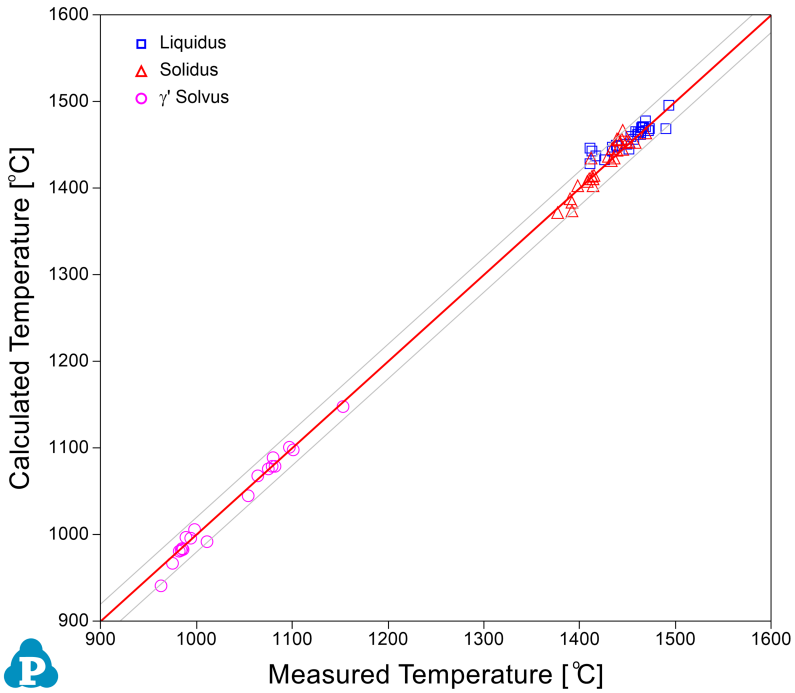


Figure 1.6: Comparison between calculated results and experimental data for Liquidus, solidus and γ' solvus temperatures

2 Mobility Database

PanCo2025_MB is an atomic mobility database for Co-based alloys, which is compatible with the `PanCo2025_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	Co	Cr	Cu	Fe	Mn	Mo	Nb	Ni	Pt	Re	Si	Ta	Ti	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, respectively.

Fcc Phase

Al-Co	Al-Cu	Al-Ni	Al-Pt	Al-Si	Al-W	Co-Cr	Co-Cu	Co-Fe	Co-Ni
Co-Pt	Cr-Fe	Cr-Ni	Cu-Fe	Cu-Si	Cu-Sn	Cu-Ti	Fe-Mn	Fe-Ni	Fe-Si
Mn-Ni	Nb-Ni	Ni-Pt	Ni-Re	Ni-Ta	Ni-Ti	Ni-W			

Al-Co-W	Al-Cr-Ni	Al-Cu-Si	Al-Mn-Ni	Al-Nb-Ni	Co-Fe-Ni
Co-Cr-Ni	Co-Cr-W	Co-Cu-Fe	Co-Cu-Ni	Co-Ni-Re	Cr-Cu-Ni
Cr-Fe-Ni	Cr-Nb-Ni	Cu-Fe-Mn	Cu-Fe-Ni	Cu-Mn-Ni	Fe-Mn-Si

Bcc phase

Al-Fe	Al-Ti	Cr-Fe	Cr-Ti	Cu-Ti	Fe-Ti	Nb-Ta	Nb-Ti	Nb-W	Nb-Zr
Ta-Ti	Ta-W	Ti-Zr							

Cr-Fe-Ni	Al-Cr-Ti	Al-Fe-Ti			

2.4 Database Validation

The simulated concentration profiles of a series of Co-based alloys are used to validate the current mobility database for Co-based alloys. A few examples of such simulation are shown below.

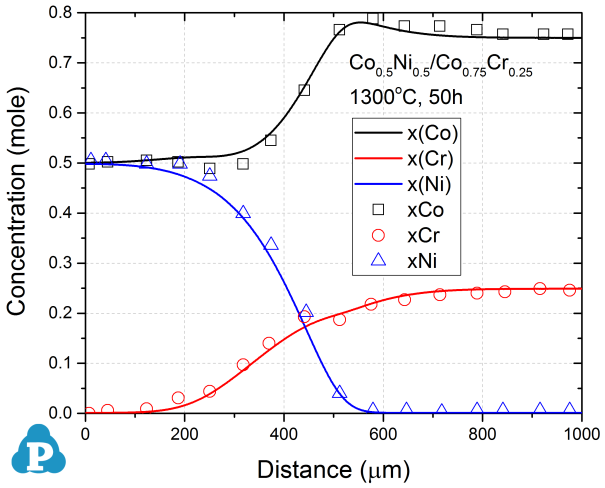


Figure 2.1: Concentration profiles of Co0.5Ni0.5/Co0.75Cr0.25 at 1300 °C for 50h [2015Che]

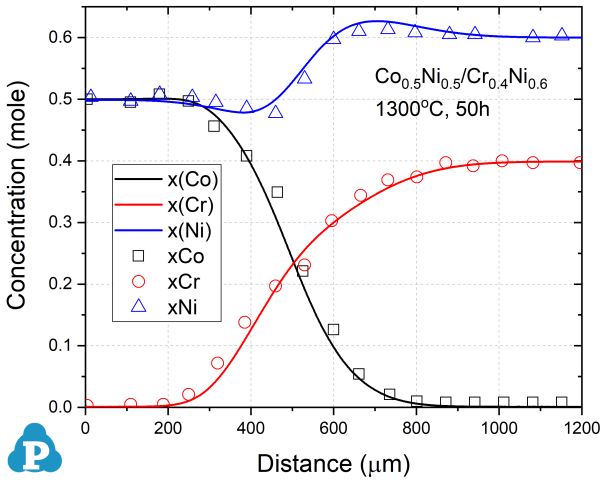


Figure 2.2: Concentration profiles of Co0.5Ni0.5/Cr0.4Ni0.6 at 1300 °C for 50h [2015Che]

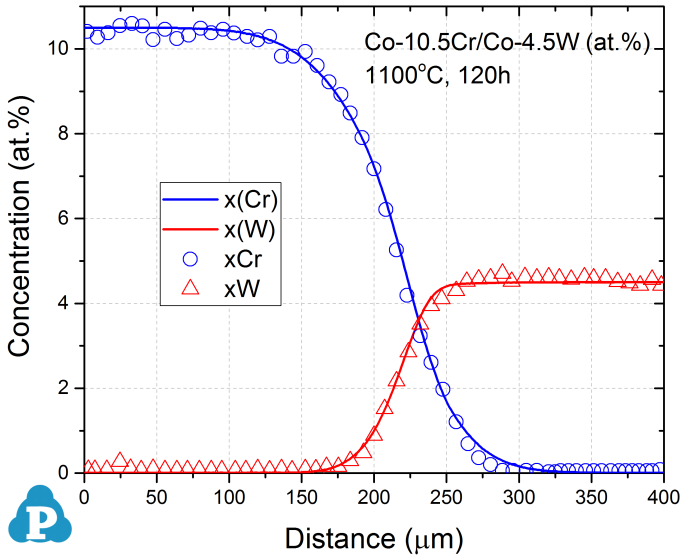


Figure 2.3: Concentration profiles of Co0.5Ni0.5/Cr0.4Ni0.6 at 1300 °C for 50h [2015Che]

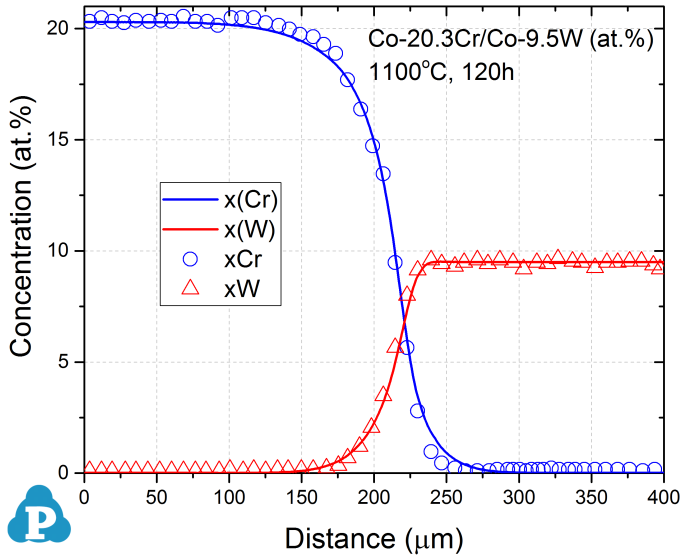


Figure 2.4: Concentration profiles of Co-20.3Cr/Co-9.5W (at.%) at 1100 °C for 120h [2014Zha]

3 Thermophysical Property Database

The thermophysical property database **PanCo2025_ TP** is compatible with the `PanCo2025_TH` thermodynamic database and suitable for the simulation of thermophysical properties of Co-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 **379** phases assessed in the `PanCo2025_TH` database. It is used to calculate the density, thermal expansion and solidification shrinkage of Co alloys.

The simulated density changes vs. temperature of a series of Co-based alloys are shown below to validate the current `PanCo2025_TP` database.

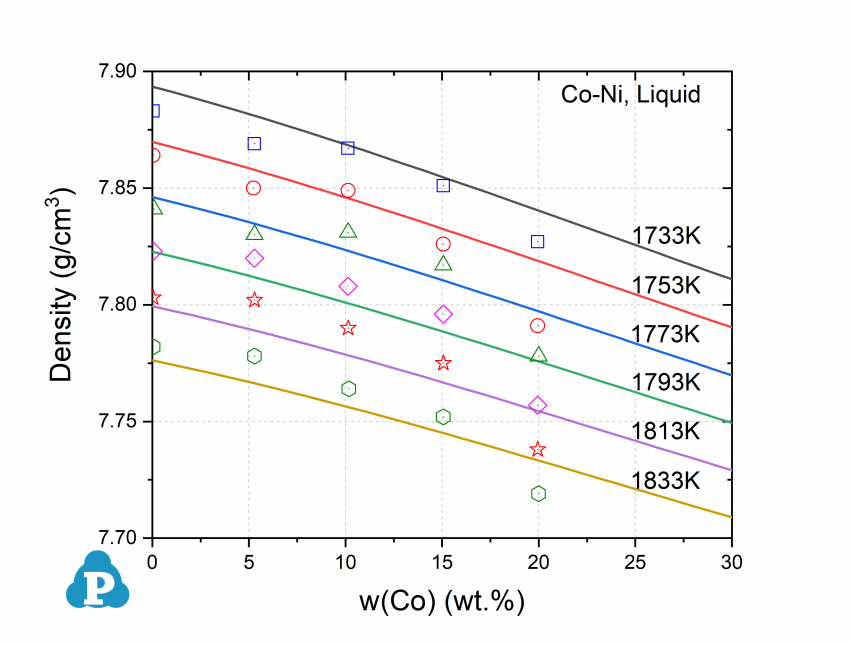


Figure 3.1: Density of Co-Ni liquid mixture [2006Fan]

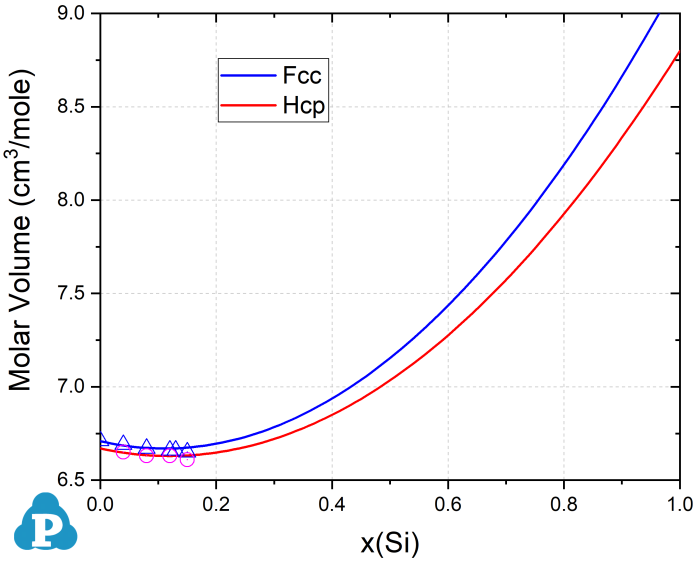


Figure 3.2: Molar volume of Co-Si Fcc and Hcp binary alloys at 298K [2006Hal]

3.2 Surface Tension

The surface tension of the liquid phase is added into the property database. 3 shows the surface tension of a series of Al-Co alloys in comparison with experimental data.

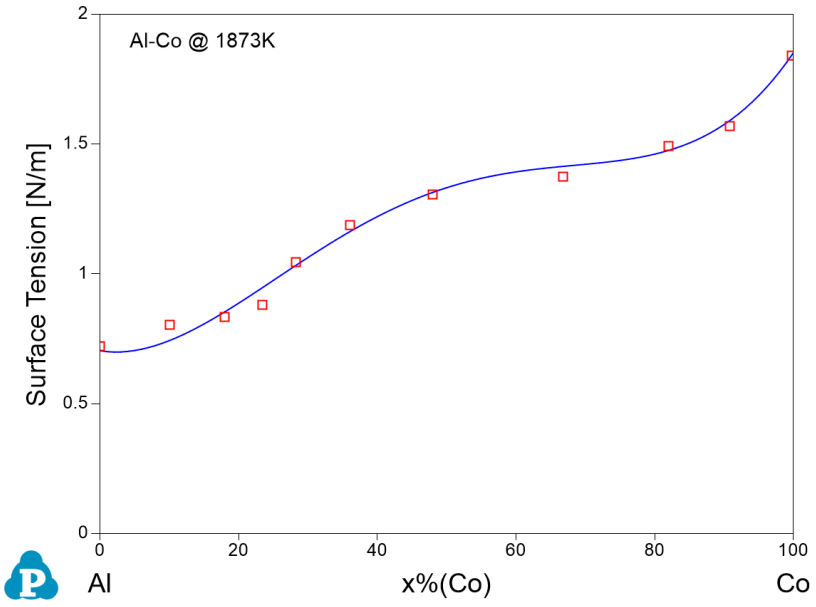


Figure 3.3: Surface tension of Al-Co alloys

3.3 Viscosity

The viscosity of the liquid phase is added into the property database. Figure 3.4 shows the viscosity of Co-Si alloy at 1873 K in comparison with experimental data.

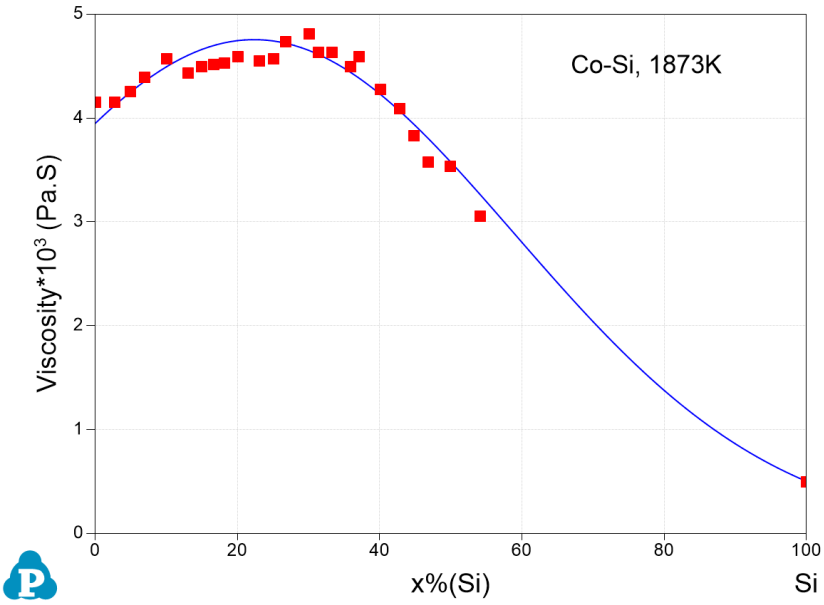


Figure 3.4: Viscosity of the Co-Si alloy at 1873 K

4 References

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PanCo2025:List of All Phases

Phases (**379**)

Name	Model	Lattice Size	Constituent
A15	CEF (SLN)	(3)(1)	(Al,Cr,Fe,Mo,Nb,Pt,Ti,V) (Al,Co,Cr,Fe,Mo,Nb,Ni,Pt,Ti,V)
A2B_oI6	CEF (SLN)	(2)(1)	(Ni,Pt)(Cr,Mo,Nb,Pt,V)
A_TiO	CEF (ST2)	(1)(1)	(Ti)(O)
Al10Fe3Ni	CEF (ST3)	(10)(3)(1)	(Al)(Fe)(Ni)
Al10FeNi3	CEF (ST3)	(10)(1)(3)	(Al)(Fe)(Ni)
Al10V	CEF (ST2)	(10)(1)	(Al)(V)
Al11Co6Si6	CEF (ST3)	(11)(6)(6)	(Al)(Co)(Si)
Al11Cr2	CEF (ST2)	(10)(1)(2)	(Al)(Al)(Cr)
Al11Mn4	CEF (SLN)	(11)(4)	(Al)(Fe,Mn)
Al11Mn4_HT	CEF (SLN)	(29)(10)	(Al,Mn)(Mn)
Al11Re4	CEF (ST2)	(11)(4)	(Al)(Re)
Al11Ti5	CEF (SLN)	(17)(8)	(Al)(Ta,Ti)
Al12M	CEF (SLN)	(12)(1)	(Al)(Fe,Mn,Mo,Re,W)
Al13Cr2	CEF (ST2)	(13)(2)	(Al)(Cr)
Al13M4	CEF (SLN)	(0.6275) (0.235) (0.1375)	(Al)(Co,Cr,Fe,Mo)(Al,Va)
Al17Mo4	CEF (SLN)	(17)(4)	(Al)(Fe,Mo)
Al1Fe1O3	CEF (ST3)	(1)(1)(3)	(Al+3)(Fe+3)(O-2)
Al21Pt5	CEF (ST2)	(21)(5)	(Al)(Pt)

Name	Model	Lattice Size	Constituent
Al21Pt8	CEF (ST2)	(21)(8)	(Al)(Pt)
Al22Mo5	CEF (SLN)	(22)(5)	(Al)(Fe,Mo)
Al23V4	CEF (ST2)	(23)(4)	(Al)(V)
Al25Co10Si7	CEF (ST3)	(25)(10)(7)	(Al)(Co)(Si)
Al2B51C8	CEF (ST3)	(2)(51)(8)	(Al)(B)(C)
Al2CoTi	CEF (SLN)	(3)(1)	(Al,Ti)(Co)
Al2Fe	CEF (SLN)	(2)(1)	(Al)(Co,Cr,Fe,Mo)
Al2Mn2Si	CEF (SLN)	(0.8)(0.2)	(Al,Mn)(Si)
Al2Mn2Si3	CEF (ST3)	(2)(2)(3)	(Al)(Mn)(Si)
Al2Pt	CEF (ST2)	(2)(1)	(Al)(Pt)
Al2Ti	CEF (SLN)	(2)(1)	(Al,Cr)(Nb,Ti)
Al2W	CEF (ST2)	(2)(1)	(Al)(W)
Al2Zr3	CEF (ST2)	(2)(3)	(Al)(Zr)
Al3B48C2	CEF (ST3)	(3)(48)(2)	(Al)(B)(C)
Al3BC	CEF (ST3)	(3)(1)(1)	(Al)(B)(C)
Al3BC3	CEF (ST3)	(3)(1)(3)	(Al)(B)(C)
Al3Co	CEF (SLN)	(3)(1)	(Al,Si)(Co)
Al3Co3Si4	CEF (ST3)	(3)(3)(4)	(Al)(Co)(Si)
Al3Mn4Si2	CEF (ST3)	(3)(4)(2)	(Al)(Mn)(Si)
Al3MnSi2	CEF (ST3)	(3)(1)(2)	(Al)(Mn)(Si)
Al3Mo	CEF (SLN)	(3)(1)	(Al)(Fe,Mo)
Al3Ni	CEF (ST2)	(0.75)(0.25)	(Al)(Ni)
Al3Ni2	CEF (SLN)	(3)(2)(1)	(Al,Si)(Al,Co,Mo,Ni) (Co,Mo,Ni,Va)
Al3Ni5	CEF (ST2)	(0.375)(0.625)	(Al)(Ni)

Name	Model	Lattice Size	Constituent
Al3Pt2	CEF (ST2)	(3)(2)	(Al)(Pt)
Al3Pt5	CEF (ST2)	(3)(5)	(Al)(Pt)
Al3SiB48	CEF (ST3)	(3)(1)(48)	(Al)(Si)(B)
Al3Zr	CEF (ST2)	(3)(1)	(Al)(Zr)
Al3Zr2	CEF (ST2)	(3)(2)	(Al)(Zr)
Al3Zr4	CEF (ST2)	(3)(4)	(Al)(Zr)
Al3Zr5	CEF (ST2)	(3)(5)	(Al)(Zr)
Al41Co33Si23	CEF (ST3)	(41)(33)(23)	(Al)(Co)(Si)
Al43Co19Si12	CEF (ST3)	(43)(19)(12)	(Al)(Co)(Si)
Al4C3	CEF (SLN)	(4)(3)	(Al,Si)(B,C)
Al4Cr	CEF (SLN)	(4)(1)	(Al)(Cr,Fe)
Al4M	CEF (SLN)	(4)(1)	(Al)(Fe,Mo,W)
Al4Mn	CEF (SLN)	(4)(1)	(Al)(Fe,Mn)
Al4Mn_L	CEF (ST2)	(461)(107)	(Al)(Mn)
Al4Re	CEF (ST2)	(4)(1)	(Al)(Re)
Al4SiC4	CEF (ST3)	(4)(1)(4)	(Al)(Si)(C)
Al4Zr5	CEF (ST2)	(4)(5)	(Al)(Zr)
Al5Co2	CEF (SLN)	(5)(2)	(Al,Si)(Co,Fe)
Al5Fe2	CEF (SLN)	(5)(2)	(Al,Fe)(Co,Cr,Fe,Mo)
Al5Fe4	CEF (SLN)	(1)	(Al,Fe,Mo)
Al5M	CEF (SLN)	(5)(1)	(Al)(Fe,Mo,W)
Al5Mn6Si7	CEF (ST3)	(5)(6)(7)	(Al)(Mn)(Si)
Al63Mo37	CEF (SLN)	(63)(37)	(Al)(Fe,Mo)
Al69Ta39	CEF (SLN)	(0.6389) (0.3611)	(Al,Ta,Ti)(Al,Ta)

Name	Model	Lattice Size	Constituent
Al6Mn	CEF (SLN)	(6)(1)	(Al)(Fe,Mn)
Al6Ni3Si	CEF (ST3)	(6)(3)(1)	(Al)(Ni)(Si)
Al6Re	CEF (ST2)	(6)(1)	(Al)(Re)
Al77W23	CEF (ST2)	(77)(23)	(Al)(W)
Al7Co4Si2	CEF (ST3)	(7)(4)(2)	(Al)(Co)(Si)
Al7V	CEF (ST2)	(7)(1)	(Al)(V)
Al7W3	CEF (ST2)	(7)(3)	(Al)(W)
Al8Cr5_H	CEF (ST2)	(8)(5)	(Al)(Cr)
Al8Cr5_L	CEF (SLN)	(8)(5)	(Al)(Cr,Fe)
Al8Mn5	CEF (SLN)	(12)(5)(9)	(Al,Si)(Mn)(Al,Fe,Mn)
Al8Mo3	CEF (SLN)	(8)(3)	(Al)(Fe,Mo)
Al8SiC7	CEF (ST3)	(8)(1)(7)	(Al)(Si)(C)
Al8V5	CEF (SLN)	(8)(5)	(Al)(Fe,Mo,V)
Al9Co2	CEF (SLN)	(9)(2)	(Al,Si)(Co)
Al9Cr4_H	CEF (ST2)	(9)(4)	(Al)(Cr)
Al9Cr4_L	CEF (SLN)	(9)(4)	(Al)(Cr,Fe)
Al9FeNi	CEF (ST3)	(9)(1)(1)	(Al)(Fe)(Ni)
AlB12	CEF (ST2)	(1)(12)	(Al)(B)
AlB40C4	CEF (ST3)	(1)(40)(4)	(Al)(B)(C)
AlCo2Nb	CEF (SLN)	(1)(2)(1)	(Al,Nb)(Co)(Al,Co,Nb)
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_	CEF (SLN)	(4)(1)(8)	(Al)(Al,Cu)(Cu)

Name	Model	Lattice Size	Constituent
H			
AlCu_Theta	CEF (SLN)	(0.667)(0.333)	(Al)(Al,Cu)
AlCu_Zeta	CEF (ST2)	(0.45)(0.55)	(Al)(Cu)
AlFeMo_Tau1	CEF (SLN)	(8)(1)(3)	(Al)(Al,Fe)(Mo)
AlFeMo_Tau2	CEF (SLN)	(1)(3)	(Al,Fe,Mo)(Va)
AlMnSi	CEF (ST3)	(1)(1)(1)	(Al)(Mn)(Si)
AlMnSi_T10	CEF (ST3)	(2)(1)(3)	(Al)(Mn)(Si)
AlMnSi_T8	CEF (SLN)	(6)(2)(12)(6)(2)	(Mn,Va)(Mn,Va)(Al)(Al,Si)(Al,Si)
AlMnSi_T9	CEF (SLN)	(14)(4)(5)	(Al)(Mn)(Al,Si)
AlNbNi2	CEF (ST3)	(0.25)(0.25)(0.5)	(Al)(Nb)(Ni)
AlNbNi_Tau2	CEF (SLN)	(1)(2)	(Nb)(Al,Ni)
AlNbNi_Tau3	CEF (SLN)	(6)(7)	(Nb)(Al,Ni)
AlNi16Si9	CEF (ST3)	(1)(16)(9)	(Al)(Ni)(Si)
AlPt	CEF (ST2)	(1)(1)	(Al)(Pt)
AlRe	CEF (ST2)	(1)(1)	(Al)(Re)
AlZr2	CEF (ST2)	(1)(2)	(Al)(Zr)
Alpha-Mn2B	CEF (ST2)	(0.670691)(0.329309)	(Mn)(B)
Alpha_B	CEF (ST1)	(1)	(B)
Alpha_Co2Si	CEF (SLN)	(2)(1)	(Co,Cr,Fe,Ni,Si)(Al,Co,Si)
Alpha_M5Si3	CEF (SLN)	(5)(3)	(Nb,Ta,W)(Si)
Alpha_MoB	CEF (SLN)	(0.5)(0.5)	(Mo,W)(B,Va)
Alpha_TiMn	CEF (ST2)	(1)(1)	(Mn)(Ti)

Name	Model	Lattice Size	Constituent
B1	CEF (SLN)	(1)(1)	(Mo,W,Zr)(B,C)
B19	CEF (SLN)	(0.5)(0.5)	(Mo,Nb,Pt,V)(Mo,Pt,V)
B2	CEF (SLN)	(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)
B2O3	CEF (ST2)	(2)(3)	(B)(O)
B3Si	CEF (SLN)	(6)(2)(6)	(B)(Si)(B,Si)
B4C	CEF (SLN)	(1)(1)	(B12,B11C)(B2,B2C,BC2,Si2)
B6Si	CEF (SLN)	(210)(23)(48)	(B)(Si)(B,Si)
BETA_VO	CEF (SLN)	(1)(1)	(V)(O,Va)
BRONZE	CEF (SLN)	(2)(5)(1)	(V+4,V+5)(O-2)(Va)
Bcc	CEF (SLN)	(1)(3)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,V,W,Zr)(B,C,O,Va)
Bcc_B2	CEF (SLN)	(0.5)(0.5)(3)	(Al,Co,Fe,Mo,Nb,Ni,Pt,Si,Ta,Ti,W,Zr)(Al,Co,Fe,Mo,Nb,Ni,Pt,Si,Ta,Ti,W,Zr)(Va)
Beta2_Ni3Si	CEF (SLN)	(3)(1)	(Ni)(Si,Ti)
Beta_B	CEF (SLN)	(93)(12)	(B)(B,Cu,Mn,Si,Zr)
Beta_Co2Si	CEF (SLN)	(2)(1)	(Co,Si)(Co,Si)
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_TiMn	CEF (ST2)	(0.515)(0.485)	(Mn)(Ti)
BnSi	CEF (SLN)	(61)(1)(8)	(B)(Si)(B,Si)
C11_b	CEF (SLN)	(2)(1)	(Co,Cr,Ni,Re,Ta)(Al,Ni,Ta)
C16	CEF (SLN)	(1)(2)	(Co,Fe,Mn,Ni,Si,Ta)

Name	Model	Lattice Size	Constituent
			(Mn,Mo,Nb,Ni,Ta,Zr)
CBCC_A12	CEF (SLN)	(1)(1)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Re,Si,Ta,Ti,V)(C,Va)
CUB_A13	CEF (SLN)	(1)(1)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Re,Si,Ta,Ti,V)(C,Va)
Cementite	CEF (SLN)	(3)(1)	(Co,Cr,Fe,Mn,Mo,Ni)(B,C)
Chi	CEF (SLN)	(24)(10)(24)	(Cr,Fe,Mo,Ni,Re)(Cr,Mo,Nb,Re,Ta,W)(Cr,Fe,Mo,Nb,Ni,Re,Ta,W)
Co11Zr2	CEF (ST2)	(11)(2)	(Co)(Zr)
Co21Cr2B6	CEF (SLN)	(21)(2)(6)	(Co,Cr)(Cr)(B)
Co23Zr6	CEF (SLN)	(23)(6)	(Co,Fe)(Zr)
Co3Si	CEF (ST2)	(0.75)(0.25)	(Co)(Si)
Co3V	CEF (ST2)	(3)(1)	(Co)(V)
Co4Cr2Ti	CEF (ST3)	(4)(2)(1)	(Co)(Cr)(Ti)
Co7Nb2	CEF (SLN)	(7)(2)	(Co)(Nb,Ti,W)
Co7Ta2	CEF (ST2)	(7)(2)	(Co)(Ta)
CoZr3	CEF (SLN)	(1)(3)	(Co,Fe)(Zr)
Corundum	CEF (SLN)	(2)(1)(3)	(Al+3,Cr+2,Cr+3,Fe+2,Fe+3,Mn+3,Ti+3,V+3,V+4,Va)(Cr+3,Fe+3,Ni+2,Va)(O-2)
Cr2B	CEF (SLN)	(0.667)(0.333)	(Co,Cr,Mo,Ni)(B)
Cr3Mn5	CEF (ST2)	(3)(5)	(Cr)(Mn)
Cr3Ni5Si2	CEF (ST3)	(3)(5)(2)	(Cr)(Ni)(Si)
Cr3Si	CEF (SLN)	(3)(1)(3)	(Cr,Mo,Nb,Ni,Si,V)(Cr,Mo,Si,V)(Va)
Cr5B3	CEF (SLN)	(0.625)(0.375)	(Cr,Mo)(B)
Cr5Ni5Si3	CEF (ST3)	(5)(5)(3)	(Cr)(Ni)(Si)

Name	Model	Lattice Size	Constituent
CrB	CEF (SLN)	(0.5)(0.5)	(Cr,Fe,Mn,Mo,Nb,Ni,W,Ta,Ti)(B,Va)
CrB4	CEF (ST2)	(0.2)(0.8)	(Cr)(B)
CrSi2	CEF (SLN)	(1)(2)	(Cr,Mo,Nb,Ta,Si,V)(Cr,Si)
Cristobalite	CEF (ST2)	(1)(2)	(Si)(O)
Cu15Si4	CEF (ST2)	(0.789474) (0.210526)	(Cu)(Si)
Cu19Si6	CEF (ST2)	(0.76)(0.24)	(Cu)(Si)
Cu2O	CEF (ST2)	(2)(1)	(Cu)(O)
Cu2Ti	CEF (ST2)	(0.666667) (0.333333)	(Cu)(Ti)
Cu33Si7	CEF (ST2)	(0.825)(0.175)	(Cu)(Si)
Cu3Ti2	CEF (ST2)	(0.6)(0.4)	(Cu)(Ti)
Cu4Ti	CEF (SLN)	(0.8)(0.2)	(Cu,Ti)(Cu,Ti)
Cu4Ti3	CEF (ST2)	(0.57143) (0.42857)	(Cu)(Ti)
Cu51Zr14	CEF (ST2)	(51)(14)	(Cu)(Zr)
Cu56Si11	CEF (ST2)	(0.835821) (0.164179)	(Cu)(Si)
Cu8Zr3	CEF (ST2)	(8)(3)	(Cu)(Zr)
CuO	CEF (ST2)	(1)(1)	(Cu)(O)
CuTi	CEF (SLN)	(0.5)(0.5)	(Cu,Ti)(Cu,Ti)
CuZr2	CEF (SLN)	(1)(2)	(Cu)(Ti,Zr)
D0_19	CEF (SLN)	(0.75)(0.25) (0.5)	(Al,Co,Cr,Mo,Nb,Ni,Pt,Ta,Ti) (Al,Co,Mo,Nb,Pt,Si,Ta,Ti,W,Zr) (C,Va)
D0_22	CEF (SLN)	(0.75)(0.25)	(Al,Cr,Ni,Pt,Si,Ti,V)

Name	Model	Lattice Size	Constituent
		(0.5)	(Al,Nb,Ni,Pt,Ta,Ti,V)(C,Va)
Delta	CEF (SLN)	(3)(1)	(Al,Co,Cr,Fe,Mo,Nb,Ni,Ta) (Al,Co,Cr,Fe,Mo,Nb,Ni,Ta,Ti)
Diamond	CEF (SLN)	(1)	(Al,B,C,Si,Ti)
Disorder	CEF (SLN)	(1)(1)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni, Pt,Re,Si,Ta,Ti,V,W,Zr)(Va)
Epsilon_Ni3Si2	CEF (SLN)	(3)(2)	(Co,Fe,Ni)(Si)
Eta	CEF (SLN)	(0.75)(0.25)	(Co,Fe,Ni,Pt,Ti,Zr) (Al,Cr,Mo,Ni,Pt,Si,Ti,Zr)
Fcc	CEF (SLN)	(1)(1)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Pt, Re,Si,Ta,Ti,V,W,Zr)(B,C,Va)
Fe2Si	CEF (ST2)	(2)(1)	(Fe)(Si)
Fe2Ta3	CEF (SLN)	(2)(3)	(Fe,Ta)(Fe,Ta)
Fe3Si7	CEF (ST2)	(0.3)(0.7)	(Fe)(Si)
Fe4Re	CEF (SLN)	(4)(1)	(Fe,Re)(Fe,Re)
Fe5Ni3Si2	CEF (SLN)	(3)(1)(1)	(Fe,Ni)(Ni)(Si)
FeSi2	CEF (SLN)	(1)(2)	(Fe,Ni)(Si)
GAS	GAS	(1)	(Al,AlO,AlO2,Al2,Al2O,Al2O2,Al2O3, C1O1,C1O2,Fe,FeO,FeO2,Fe2,Mn, O,O2,O3,Si,Si2,Si3,SiO,SiO2,Ti,TiO, TiO2,Zr,Zr2,ZrO,ZrO2)
Gamma_Ni5Si2	CEF (SLN)	(5)(2)	(Co,Cr,Fe,Ni)(Al,Si)
Graphite	CEF (SLN)	(1)	(B,C)
H_Sigma_CrMn	CEF (SLN)	(8)(4)(18)	(Fe,Mn)(Cr)(Cr,Fe,Mn)
H_Ti2AlC	CEF (SLN)	(2)(1)(1)	(Ti)(Al)(C,Va)
Halite	CEF (SLN)	(1)(1)	(Al+3,Co+2,Cr+3,Fe+2,Fe+3,Mn+2,

Name	Model	Lattice Size	Constituent
			Mn+3,Ni+2,V,V+2,V+3,Va)(O-2,Va)
Hcp	CEF (SLN)	(1)(0.5)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,V,W,Zr)(B,C,O,Va)
L10	CEF (SLN)	(0.5)(0.5)(1)	(Al,Co,Cr,Fe,Mn,Ni,Pt,Ti) (Al,Co,Cr,Fe,Mn,Ni,Pt,Ti)(Va)
L10_TiAl	CEF (SLN)	(1)(1)(2)	(Al,Cr,Mo,Nb,Ta,Ti) (Al,Cr,Mo,Nb,Ta,Ti)(C,Va)
L11	CEF (SLN)	(0.5)(0.5)(1)	(Cu,Pt)(Cu,Pt)(Va)
L12	CEF (SLN)	(0.75)(0.25)(1)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,V,W,Zr)(Al,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Pt,Re,Si,Ta,Ti,V,W,Zr)(Va)
Laves_C14	CEF (SLN)	(2)(1)	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Re,Si,Ta,Ti,V,Zr)(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Ta,Ti,V,W,Zr)
Laves_C15	CEF (SLN)	(2)(1)	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Ta,Ti,V,W,Zr) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ta,Ti,V,W,Zr)
Laves_C36	CEF (SLN)	(2)(1)	(Al,Co,Cr,Fe,Mn,Ni,Ta,Ti,Zr) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ta,Ti,Zr)
Liquid	CEF (SLN)	(1)	(Al,B,C,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,O,Pt,Re,Si,Ta,Ti,V,W,Zr,Al2O3,B2O3,CoO,Co2O3,Cr2/3O,CuO,Cu2O,Cu2O3,FeO,FeO3/2,MnO,MnO3/2,MoO2,MoO3,NbO,NbO2,NbO5/2,NiO,SiO2,Ta2O5,TiO,TiO3/2,TiO2,VO,VO2,VO3/2,VO5/2,WO2,WO3,Zr1/2O)
M12C	CEF (SLN)	(6)(6)(1)	(Co,Ni)(Mo,W)(C)

Name	Model	Lattice Size	Constituent
M23C6	CEF (SLN)	(20)(3)(6)	(Co,Cr,Fe,Mn,Mo,Ni,Re) (Co,Cr,Fe,Mn,Mo,Ni,Re,Ta,W)(C)
M2B	CEF (SLN)	(2)(1)	(Co,Cr,Fe,Mn,Mo,Ni,Ta,W)(B)
M2O3_cI80	CEF (SLN)	(2)(3)(1)	(Mn+3,Va)(O-2)(O-2,Va)
M2SiO4	CEF (SLN)	(2)(1)	(FeO,MnO,NiO)(SiO2)
M3AlC	CEF (SLN)	(3)(1)(1)	(Al,Co,Ni,Fe)(Al,Co,Ni,Fe)(C)
M3B2	CEF (SLN)	(0.6)(0.4)	(Cr,Mo,Nb,Ta,V)(B)
M3B4	CEF (SLN)	(3)(4)	(Cr,Mn,Mo,Nb,Ta,Ti,V)(B)
M3C2	CEF (SLN)	(3)(2)	(Co,Cr,Mo,V,W)(C)
M3Si	CEF (SLN)	(3)(1)	(Mo,Nb,Ta,Ti,Zr)(Si)
M3Ti	CEF (SLN)	(3)(1)	(Co,Ni)(Co,Ni,Ti)
M4Si3	CEF (SLN)	(4)(3)	(Cr,Ni)(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)
M5Zr	CEF (SLN)	(5)(1)	(Cu,Ni)(Zr)
M6C	CEF (SLN)	(2)(2)(2)(1)	(Co,Fe,Ni)(Cr,Mo,Nb,Ta,W) (Co,Cr,Fe,Mo,Nb,Ni,Ta,W)(C)
M7C3	CEF (SLN)	(7)(3)	(Co,Cr,Fe,Mn,Mo,Ni,Re,W)(C)
MB	CEF (SLN)	(1)(1)	(Co,Fe,Mn,Ni,Ti)(B,C)
MB2	CEF (SLN)	(1)(2)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,V,Zr,Va) (B,C,Va)
MO2_cF12	CEF (SLN)	(1)(2)	(Zr)(O,Va)
MO2_mP12	CEF (SLN)	(1)(2)	(Mo,V,W,Zr)(O)
MO2_tP6	CEF (SLN)	(1)(2)	(Zr)(O,Va)
MSi	CEF (SLN)	(1)(1)	(Co,Cr,Fe,Mn,Ni,Re,Si)(Al,Co,Si)
MSi2	CEF (SLN)	(1)(2)	(Mo,Nb,Re,W)(Si,Va)

Name	Model	Lattice Size	Constituent
MZr	CEF (SLN)	(1)(1)	(Al,Ni,Pt,Zr)(Pt,Zr)
Mn11Si19	CEF (SLN)	(11)(19)	(Mn)(Al,Si)
Mn3Si	CEF (SLN)	(3)(1)	(Mn,Ni)(Al,Si,Ti)
Mn3Ti	CEF (ST2)	(3)(1)	(Mn)(Ti)
Mn4Ti	CEF (ST2)	(0.815)(0.185)	(Mn)(Ti)
Mn5C2	CEF (SLN)	(5)(2)	(Fe,Mn)(C)
Mn5Si3	CEF (SLN)	(2)(3)(3)(1)	(Fe,Mn,Ni,Si,Ti,Zr)(Al,Ni,Si,Ti) (Fe,Mn,Ti,Zr)(C,Va)
Mn6Si	CEF (SLN)	(17)(3)	(Mn)(Al,Si)
Mn9Si2	CEF (ST2)	(33)(7)	(Mn)(Si)
MnB4	CEF (ST2)	(0.2)(0.8)	(Mn)(B)
MnNi2	CEF (SLN)	(1)(2)	(Mn,Ni)(Ni)
MnNiSi_T1	CEF (ST3)	(0.15)(0.45) (0.4)	(Mn)(Ni)(Si)
MnNiSi_T10	CEF (ST3)	(0.66)(0.04) (0.3)	(Mn)(Ni)(Si)
MnNiSi_T11	CEF (ST3)	(0.52)(0.29) (0.19)	(Mn)(Ni)(Si)
MnNiSi_T12	CEF (SLN)	(3)(1)	(Mn,Ni)(Si)
MnNiSi_T2	CEF (ST3)	(0.15)(0.5) (0.35)	(Mn)(Ni)(Si)
MnNiSi_T3	CEF (ST3)	(0.206897) (0.551724) (0.241379)	(Mn)(Ni)(Si)
MnNiSi_T4	CEF (ST3)	(0.333333) (0.333333) (0.333334)	(Mn)(Ni)(Si)

Name	Model	Lattice Size	Constituent
MnNiSi_T5	CEF (SLN)	(1)(2)	(Mn)(Ni,Si)
MnNiSi_T6	CEF (SLN)	(1)(2)	(Mn)(Ni,Si)
MnNiSi_T7	CEF (ST3)	(0.5) (0.333333) (0.166667)	(Mn)(Ni)(Si)
MnNiSi_T8	CEF (SLN)	(3)(1)	(Mn,Ni)(Si)
MnNiSi_T9	CEF (ST3)	(0.61)(0.12) (0.27)	(Mn)(Ni)(Si)
Mo2B5	CEF (SLN)	(2)(5)	(Mo,W)(B,Va)
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)
MoO3	CEF (ST2)	(1)(3)	(Mo)(O)
MoPt2	CEF (SLN)	(0.3333) (0.6667)	(Mo,Pt)(Mo,Pt)
Mu	CEF (SLN)	(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)
N8M	CEF (SLN)	(8)(1)	(Al,Co,Ni,Pt)(Mo,Nb,Ta,Ti)
N_Ti3AlC2	CEF (SLN)	(3)(1)(2)	(Ti)(Al)(C,Va)
Nb2B3	CEF (ST2)	(2)(3)	(Nb)(B)

Name	Model	Lattice Size	Constituent
Nb2O5	CEF (ST2)	(2)(5)	(Nb)(O)
Nb5B6	CEF (ST2)	(5)(6)	(Nb)(B)
NbO	CEF (ST2)	(1)(1)	(Nb)(O)
NbO2	CEF (ST2)	(1)(2)	(Nb)(O)
NbPt3	CEF (ST2)	(1)(3)	(Nb)(Pt)
Ni10Zr7	CEF (SLN)	(10)(7)	(Cu,Ni,Pt)(Zr)
Ni11Zr9	CEF (ST2)	(11)(9)	(Ni)(Zr)
Ni16Si7Ti6	CEF (SLN)	(16)(7)(6)	(Co,Ni)(Si)(Si,Ti)
Ni21Zr8	CEF (ST2)	(21)(8)	(Ni)(Zr)
Ni2AlSi	CEF (SLN)	(1)(1)	(Ni)(Al,Si,Va)
Ni2AlTa	CEF (ST3)	(2)(1)(1)	(Ni)(Al)(Ta)
Ni2SiO4	CEF (ST3)	(2)(1)	(NiO)(SiO2)
Ni3Ta	CEF (SLN)	(3)(1)	(Co,Mn,Mo,Ni,Ta)(Al,Mo,Ni,Ta)
Ni4M	CEF (SLN)	(4)(1)	(Ni)(Mo,W)
Ni4Si3Ti	CEF (SLN)	(4)(3)(1)	(Ni,Ti)(Si)(Ti)
Ni4Si7Ti4	CEF (SLN)	(4)(7)(4)	(Ni)(Si,Ti)(Si,Ti)
Ni6AlTa	CEF (SLN)	(3)(0.5)(0.5)	(Ni)(Al,Ni)(Ta)
Ni7Zr2	CEF (SLN)	(7)(2)	(Al,Ni)(Zr)
NiMo	CEF (SLN)	(24)(20)(12)	(Co,Cr,Fe,Ni) (Al,Co,Cr,Fe,Mn,Mo,Ni,Ta,W) (Mo,Re,Ta,W)
NiSi	CEF (SLN)	(1)(1)	(Co,Fe,Ni,Pt,Ti,Zr)(Al,Si)
NiSi2	CEF (SLN)	(1)(2)	(Co,Fe,Mn,Ni)(Al,Si)
NiSi4Ti4	CEF (ST3)	(1)(4)(4)	(Ni)(Si)(Ti)
NiSiTi	CEF (SLN)	(1)(1)(1)	(Ni,Ti)(Si)(Ni,Ti)

Name	Model	Lattice Size	Constituent
NiTi2	CEF (SLN)	(1)(2)	(Co,Cr,Fe,Ni)(Al,Nb,Ti)
NiW2	CEF (SLN)	(1)(2)	(Co,Ni)(W)
P_Phase	CEF (SLN)	(24)(12)(20)	(Cr,Fe,Ni)(Mo)(Cr,Mo,Ni)
P_Ti3AlC	CEF (SLN)	(3)(1)(1)	(Ti)(Al,Ti)(C,Va)
Phi	CEF (SLN)	(0.8837) (1.1163)	(Al,Ta,Ti)(Al,Ta,Ti)
Pt17Si8_alpha	CEF (ST2)	(0.68)(0.32)	(Pt)(Si)
Pt17Si8_beta	CEF (ST2)	(0.68)(0.32)	(Pt)(Si)
Pt25Si7	CEF (ST2)	(0.782)(0.218)	(Pt)(Si)
Pt2B	CEF (ST2)	(2)(1)	(Pt)(B)
Pt2Si_alpha	CEF (ST2)	(0.667)(0.333)	(Pt)(Si)
Pt2Si_beta	CEF (ST2)	(0.667)(0.333)	(Pt)(Si)
Pt2Ta	CEF (ST2)	(2)(1)	(Pt)(Ta)
Pt3B	CEF (ST2)	(3)(1)	(Pt)(B)
Pt3B2	CEF (ST2)	(3)(2)	(Pt)(B)
Pt3Si_alpha	CEF (ST2)	(3)(1)	(Pt)(Si)
Pt3Si_beta	CEF (ST2)	(3)(1)	(Pt)(Si)
Pt3Zr5	CEF (SLN)	(3)(5)	(Pt,Zr)(Pt,Zr)
Pt4Zr	CEF (SLN)	(4)(1)	(Pt,Zr)(Pt,Zr)
Pt4Zr3	CEF (SLN)	(4)(3)	(Pt,Zr)(Pt,Zr)
Pt5Si2	CEF (ST2)	(0.714)(0.286)	(Pt)(Si)
Pt6Si5	CEF (ST2)	(0.545)(0.455)	(Pt)(Si)
PtO2	CEF (ST2)	(1)(2)	(Pt)(O)
PtTa	CEF (ST2)	(1)(1)	(Pt)(Ta)
PtTa6	CEF (ST2)	(1)(6)	(Pt)(Ta)

Name	Model	Lattice Size	Constituent
Quartz	CEF (ST2)	(1)(2)	(Si)(O)
R_Phase	CEF (SLN)	(27)(14)(12)	(Co,Cr,Fe,Mo,W)(Cr,Mo,W) (Co,Cr,Fe,Mo,W)
Re24Ti5	CEF (SLN)	(24)(5)	(Re)(Ti,Zr)
Re25Zr21	CEF (ST2)	(0.5435) (0.4565)	(Re)(Zr)
Re2O7	CEF (ST2)	(2)(7)	(Re)(O)
Re2Si	CEF (ST2)	(2)(1)	(Re)(Si)
Re3B	CEF (ST2)	(0.75)(0.25)	(Re)(B)
Re7B3	CEF (ST2)	(0.7)(0.3)	(Re)(B)
ReB2	CEF (SLN)	(1)(2)	(B,Re)(B)
ReO2	CEF (ST2)	(1)(2)	(Re)(O)
ReO3	CEF (ST2)	(1)(3)	(Re)(O)
Rutile	CEF (SLN)	(1)(2)	(Mn+4,Ti+3,Ti+4,V+4)(O-2,Va)
Si2Zr	CEF (ST2)	(2)(1)	(Si)(Zr)
Si2Zr3	CEF (ST2)	(2)(3)	(Si)(Zr)
Si5V6	CEF (ST2)	(0.454545) (0.545455)	(Si)(V)
SiC	CEF (SLN)	(1)(1)	(Si)(B,C)
SiO_AM	CEF (ST2)	(1)(1)	(Si)(O)
Sigma	CEF (SLN)	(8)(4)(18)	(Al,Co,Cr,Fe,Mn,Ni,Pt,Re,Ta,W) (Cr,Fe,Mo,Nb,Re,Ta,Ti,V,W) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Pt,Re, Si,Ta,Ti,V,W)
Spinel	CEF (SLN)	(1)(2)(2)(4)	(Al+3,Co+2,Cr+2,Cr+3,Fe+2,Fe+3, Mn+2,Ni+2)(Al+3,Co+3,Cr+3,Fe+2,

Name	Model	Lattice Size	Constituent
			Fe+3,Mn+2,Mn+3,Mn+4,Ni+2,Va) (Fe+2,Va)(O-2)
Spinel_T	CEF (SLN)	(1)(2)(2)(4)	(Cr+2,Cr+3,Fe+2,Fe+3,Mn+2,Mn+3) (Cr+3,Fe+2,Fe+3,Mn+2,Mn+3,Va) (Fe+2,Va)(O-2)
Ta2O5_S	CEF (SLN)	(1)	(Ta,Ta2O5)
Ta2O5_S2	CEF (SLN)	(1)	(Ta,Ta2O5)
Theta_Ni2Si	CEF (SLN)	(1)(1)(1)	(Fe,Ni)(Cr,Fe,Ni,Va)(Al,Si)
Ti10O19	CEF (ST2)	(10)(19)	(Ti)(O)
Ti20O39	CEF (ST2)	(20)(39)	(Ti)(O)
Ti31Al19Si50	CEF (SLN)	(1)(2)	(Ti)(Al,Si)
Ti3O2	CEF (ST2)	(3)(2)	(Ti)(O)
Ti3O5	CEF (ST2)	(3)(5)	(Ti)(O)
Ti3SiC2	CEF (ST3)	(3)(1)(2)	(Ti)(Si)(C)
Ti4O7	CEF (ST2)	(4)(7)	(Ti)(O)
Ti4Pt3	CEF (ST2)	(3)(4)	(Pt)(Ti)
Ti5O9	CEF (ST2)	(5)(9)	(Ti)(O)
Ti6O11	CEF (ST2)	(6)(11)	(Ti)(O)
Ti6Si2B	CEF (ST3)	(6)(2)(1)	(Ti)(Si)(B)
Ti7Al5Si12	CEF (SLN)	(7)(1)(16)	(Ti)(Al)(Al,Si)
Ti7O13	CEF (ST2)	(7)(13)	(Ti)(O)
Ti8O15	CEF (ST2)	(8)(15)	(Ti)(O)
Ti9O17	CEF (ST2)	(9)(17)	(Ti)(O)
TiOx	CEF (SLN)	(1)(1)(1)	(Ti+2,Ti+3,Va)(Ti,Va)(O-2)
TiPt3	CEF (SLN)	(1)(3)	(Pt,Ti)(Pt)

Name	Model	Lattice Size	Constituent
TiPt_alpha	CEF (SLN)	(1)(1)	(Pt,Ti)(Pt,Ti)
TiPt_beta	CEF (SLN)	(1)(1)	(Pt,Ti)(Pt,Ti)
TiSi2	CEF (SLN)	(1)(2)	(Ti)(Al,Si)
Tridymite	CEF (ST2)	(1)(2)	(Si)(O)
V2B3	CEF (ST2)	(2)(3)	(V)(B)
V2O5	CEF (ST2)	(2)(5)	(V)(O)
V2O_SS	CEF (SLN)	(1)(0.5)	(V)(O,Va)
V3O5_HT	CEF (ST2)	(2)(1)(5)	(V+3)(V+4)(O-2)
V3O5_LT	CEF (ST2)	(2)(1)(5)	(V+3)(V+4)(O-2)
V3O7	CEF (ST2)	(2)(1)(7)	(V+5)(V+4)(O-2)
V4O7	CEF (ST2)	(2)(2)(7)	(V+3)(V+4)(O-2)
V52O64	CEF (ST2)	(52)(64)	(V)(O)
V5B6	CEF (ST2)	(5)(6)	(V)(B)
V5O9	CEF (ST2)	(2)(3)(9)	(V+3)(V+4)(O-2)
V6O11	CEF (ST2)	(2)(4)(11)	(V+3)(V+4)(O-2)
V6O13	CEF (ST2)	(2)(4)(13)	(V+5)(V+4)(O-2)
V7O13	CEF (ST2)	(2)(5)(13)	(V+3)(V+4)(O-2)
V8O15	CEF (ST2)	(2)(6)(15)	(V+3)(V+4)(O-2)
VB	CEF (ST2)	(1)(1)	(V)(B)
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)

Name	Model	Lattice Size	Constituent
Y2O3_hex	CEF (SLN)	(2)(3)(1)	(Zr+4)(O-2)(O-2,Va)
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)
ZrB12	CEF (ST2)	(1)(12)	(Zr)(B)
alpha-NbPt	CEF (ST2)	(43)(57)	(Nb)(Pt)
m_Ni4B3	CEF (ST2)	(0.564)(0.436)	(Ni)(B)
o_Ni4B3	CEF (ST2)	(0.586)(0.414)	(Ni)(B)