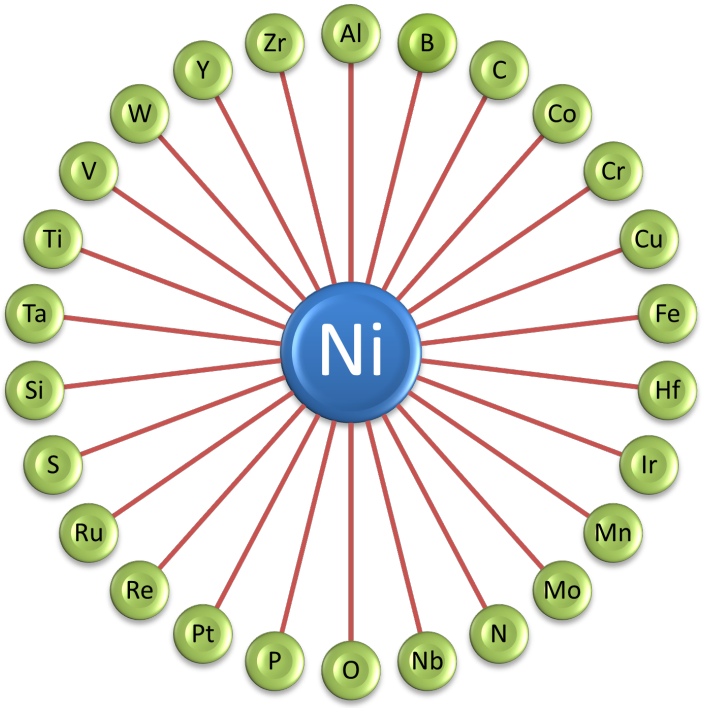
Pandat 2025

Database Manual

CompuTherm LLC

PanNickel

Database for multi-component Nickel-based Superalloys



PANDAT™
SOFTWARE

Contents

1 Thermodynamic Database

1.1 Components (27)

A total of **27** components are included in the database as listed here:

Al-B-C-Co-Cr-Cu-Fe-Hf-Ir-Mn-Mo-N-Nb-**Ni**-O-P-Pt-Re-Ru-S-Si-Ta-Ti-V-W-Y-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 1.5 .

Table 1.1: Suggested composition range

Elements	Composition Range (wt.%)
Ni	50-100
Pt	0-40
Al,Co,Cr,Fe	0-22
Ir,Mo,Re,Ru,Ta,V,W	0-12
Hf,Nb,Ti	0-5
B,C,Cu,Mn,N,O,Si,Y,Zr	0-0.5
P,S	0-0.01

1.3 What is new in PanNi2025

Some of Nb-related ternary systems are updated, including C-Nb-Ti, Co-Nb-Ni, Fe-Nb-Ti, Fe-Ni-Ti ternary systems.

1.4 Phases

Total of **343** 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 PanNi2025: List of 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,Fe,Hf,Ir,Mn,Mo,Nb,Ni,Pt,Re,Ru,Si, Ta,Ti,V,W,Zr) (Al,Co,Cr,Cu,Fe,Hf,Ir,Mn,Mo,Nb, Ni,Pt,Re,Ru,Si,Ta,Ti,V,W,Va)
Bcc	(1)(3)	(Al,Co,Cr,Cu,Fe,Hf,Ir,Mn,Mo,Nb,Ni,P,Pt, Re,Ru,S,Si,Ta,Ti, V,W,Y,Zr) (B,C,N,O,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,Nb,Ni,Re,Ta,Ti) (Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Si,Ta,Ti,W,Zr)
Eta	(0.75)(0.25)	(Co,Cu,Fe,Ni,Ti)(Al,Cr,Hf,Mo,Nb,Ni,Si,Ta,Ti,V,Zr)
Fcc	(1)(1)	(Al,Co,Cr,Cu,Fe,Hf,Ir,Mn,Mo,Nb,Ni,P,Pt,Re,Ru, S,Si,Ta,Ti, V,W,Y,Zr)(B,C,N,O,Va)
Fcc_MC	(1)(1)	(Co,Cr,Fe,Hf,Mo,Nb,Ni,Si,Ta,Ti,W,Zr)(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,V,W,Y,Zr) (Al,Co,Cr,Fe,Hf,Ir,Mn,Mo,Nb,Ni,Pt, Re,Ru,Si,Ta,Ti,V,W,Y,Zr) (Va)
Laves_C14	(2)(1)	(Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Si,Ta,Ti,V,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,V,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,O,P,Pt, Re,Ru,S,Si,Ta,Ti,V,W,Y,Zr,Co2P,Cu3P,Al2S3,

Name	Lattice Size	Constituent
		Cr1S1,Fe1S1,Mo2S3,Ni1S1,Mn1S1,Al2O3,B2O3, CoO,Co2O3,Cr2/3O,CuO,Cu2O,Cu2O3,FeO,FeO3/2, HfO2,MnO,Mn2/3O,MoO2,MoO3,NbO,NbO2,Nb2O5, NiO,P,P4O10,P4O6,SO3,SiO2,Ta2O5,TiO,TiO3/2, TiO2,VO,VO2,VO3/2,VO5/2,WO2,WO3,Y2O3,Zr1/2O)
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)
Sigma	(8)(4)(18)	(Al,Co,Fe,Mn,Ni,Re,Ru,Si)(Co,Cr,Mo,Nb,Ni,Ta,Ti,V,W) (Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Re,Ru,Si,Ta,Ti,V,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 Assessed Subsystems

A total of **314** subsystems, including 241 binary and 73 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 (241)

Al-B(10)	Al-C(10)	Al-Co(10)	Al-Cr(10)	Al-Fe(6)	Al-Hf(10)	Al-Ir(10)
Al-Mn(10)	Al-Mo(8)	Al-Nb(10)	Al-Ni(10)	Al-O(10)	Al-Pt(10)	Al-Re(10)
Al-Ru(10)	Al-S(10)	Al-Si(10)	Al-Ta(10)	Al-Ti(10)	Al-V(10)	Al-W(6)
Al-Y(10)	Al-Zr(10)	B-Co(10)	B-Cr(10)	B-Fe(10)	B-Hf(10)	B-Mo(10)
B-Nb(10)	B-Ni(10)	B-O(10)	B-Re(10)	B-Ta(10)	B-Ti(10)	B-V(10)
B-W(10)	B-Zr(10)	C-Cr(10)	C-Fe(10)	C-Hf(10)	C-Mo(10)	C-Nb(10)
C-Ni(10)	C-Re(6)	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-Hf(10)	Co-Mn(10)	Co-Mo(10)	Co-Nb(10)
Co-Ni(10)	Co-O(10)	Co-P(10)	Co-Pt(6)	Co-Si(10)	Co-Ta(10)	Co-Ti(10)

Co-V(10)	Co-W(10)	Co-Y(10)	Co-Zr(10)	Cr-Cu(10)	Cr-Fe(10)	Cr-Hf(10)
Cr-Ir(10)	Cr-Mn(10)	Cr-Mo(10)	Cr-N(10)	Cr-Nb(10)	Cr-Ni(10)	Cr-O(10)
Cr-P(10)	Cr-Pt(10)	Cr-Re(10)	Cr-Ru(10)	Cr-S(10)	Cr-Si(10)	Cr-Ta(10)
Cr-Ti(10)	Cr-V(10)	Cr-W(10)	Cr-Y(10)	Cr-Zr(10)	Cu-Fe(10)	Cu-Ir(10)
Cu-Mn(10)	Cu-Nb(10)	Cu-Ni(10)	Cu-O(10)	Cu-P(10)	Cu-Si(10)	Cu-Ta(10)
Cu-Ti(10)	Cu-V(10)	Cu-W(10)	Cu-Y(10)	Cu-Zr(10)	Fe-Hf(10)	Fe-Ir(10)
Fe-Mn(10)	Fe-Mo(10)	Fe-N(10)	Fe-Nb(10)	Fe-Ni(10)	Fe-O(10)	Fe-P(10)
Fe-Pt(6)	Fe-Re(10)	Fe-S(10)	Fe-Si(10)	Fe-Ta(10)	Fe-Ti(10)	Fe-V(10)
Fe-W(10)	Fe-Y(10)	Fe-Zr(10)	Hf-Mn(10)	Hf-Mo(10)	Hf-N(10)	Hf-Nb(10)
Hf-Ni(10)	Hf-O(10)	Hf-Si(10)	Hf-Ta(10)	Hf-Ti(10)	Hf-V(10)	Hf-W(10)
Hf-Y(10)	Ir-Ni(10)	Ir-O(10)	Ir-Pt(10)	Ir-Y(10)	Mn-Mo(10)	Mn-Nb(10)
Mn-Ni(10)	Mn-O(10)	Mn-P(10)	Mn-Pt(10)	Mn-S(10)	Mn-Si(10)	Mn-Ta(10)
Mn-Ti(10)	Mn-V(10)	Mn-W(10)	Mn-Y(10)	Mn-Zr(10)	Mo-N(10)	Mo-Nb(10)
Mo-Ni(10)	Mo-O(10)	Mo-P(10)	Mo-Pt(10)	Mo-Re(10)	Mo-Ru(10)	Mo-S(10)
Mo-Si(10)	Mo-Ti(10)	Mo-V(10)	Mo-W(10)	Mo-Y(10)	Mo-Zr(10)	N-Nb(10)
N-Ni(10)	N-Ta(10)	N-Ti(10)	N-V(10)	N-W(10)	N-Zr(10)	Nb-Ni(10)
Nb-O(10)	Nb-P(10)	Nb-Si(10)	Nb-Ti(10)	Nb-V(10)	Nb-W(10)	Nb-Y(10)
Nb-Zr(10)	Ni-O(10)	Ni-P(10)	Ni-Pt(10)	Ni-Re(10)	Ni-Ru(10)	Ni-S(10)
Ni-Si(10)	Ni-Ta(10)	Ni-Ti(10)	Ni-V(10)	Ni-W(10)	Ni-Y(10)	Ni-Zr(10)
O-P(10)	O-Pt(10)	O-Ru(10)	O-Si(10)	O-Ta(10)	O-Ti(10)	O-V(10)
O-W(10)	O-Y(10)	O-Zr(10)	P-Ti(10)	Pt-Si(10)	Pt-Ta(10)	Pt-V(10)
Pt-Y(10)	Pt-Zr(10)	Re-Si(10)	Re-Ta(10)	Re-W(10)	Re-Y(10)	Re-Zr(10)
Ru-Si(10)	Ru-Ta(10)	Ru-Y(10)	S-Ti(10)	Si-Ta(10)	Si-Ti(10)	Si-V(10)
Si-W(10)	Si-Y(10)	Si-Zr(10)	Ta-Ti(10)	Ta-V(10)	Ta-W(10)	Ta-Y(10)
Ta-Zr(10)	Ti-V(10)	Ti-W(10)	Ti-Y(10)	Ti-Zr(10)	V-W(10)	V-Y(10)
V-Zr(10)	W-Zr(10)	Y-Zr(10)				

Ternary Systems (73)

Al-B-Cr(6)	Al-B-Ni(6)	Al-Co-Ni(10)	Al-Co-W(10)	Al-Cr-Ni(10)	Al-Mo-Ni(8)
Al-Nb-Ni(8)	Al-Ni-Pt(8)	Al-Ni-Re(8)	Al-Ni-Si(8)	Al-Ni-Ta(8)	Al-Ni-Ti(8)
Al-Ni-W(8)	B-Co-Cr(6)	B-Co-Ni(6)	B-Cr-Fe(6)	B-Cr-Ti(6)	B-Fe-Ni(6)
B-Ni-Ti(6)	B-Ni-W(6)	C-Co-Cr(6)	C-Co-Fe(6)	C-Co-Ni(6)	C-Co-W(6)
C-Cr-Ni(6)	C-Cr-Ti(6)	C-Fe-Ni(6)	C-Fe-W(6)	C-Mo-Ti(6)	C-Mo-W(6)
C-Nb-Ti(6)	C-Nb-W(6)	C-Ni-W(6)	Co-Cr-Mo(8)	Co-Cr-Ni(8)	Co-Cr-Ti(8)
Co-Cr-W(8)	Co-Fe-W(8)	Co-Mo-Ni(8)	Co-Nb-Ni(8)	Co-Ni-Si(8)	Co-Ni-Ta(8)
Co-Ni-Ti(8)	Co-Ni-W(8)	Cr-Fe-Ni(8)	Cr-Fe-Ti(8)	Cr-Mo-Nb(8)	Cr-Mo-Ni(8)
Cr-Nb-Ni(8)	Cr-Ni-Pt(8)	Cr-Ni-Ru(8)	Cr-Ni-Ta(8)	Cr-Ni-Ti(8)	Cr-Ni-W(8)
Cu-Hf-Ni(8)	Cu-Nb-Ni(8)	Cu-Ni-Si(8)	Cu-Ni-Ta(8)	Cu-Ni-Ti(8)	Cu-Ni-Zr(8)
Fe-Mo-Ni(8)	Fe-Nb-Ni(8)	Fe-Nb-Ti(8)	Fe-Ni-Si(8)	Fe-Ni-Ti(8)	Fe-Ni-W(8)
Mo-Nb-Ni(8)	Mo-Ni-Si(8)	Mo-Ni-Ta(8)	Mo-Ni-W(8)	Nb-Ni-Ti(8)	Ni-Si-Ti(8)
Ni-Ti-W(8)					

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 1.3 lists the alloys and references used for testing the current database. In the table, T^{l}, T^{s}, and $T^{\gamma'}$ represent liquidus(γ starts to form from liquid), solidus (all liquid disappears), 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 γ , x(X) in γ' 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 1.3: Experimental Data Used for Testing the Current Nickel Database

Alloy	Experimental Information	References
Udimet-700	$T^{\gamma'}$, $f^{\gamma'}$ *vs.* T, x(Al,Cr,Ti,Mo,W) in γ' *vs.* T	[1971Mol]
Ni-14Cr-6.5~12Al-4Ti-1~5Mo	$T^{\gamma'}$	[1972Loo]
Ni-4~13Al-6.5~20.5Cr-0.25~4.5Ti-0~6Mo-0~4W	$f^{\gamma'}$ at 850 °C x(Al,Cr,Ti,Mo,W) in γ and γ'	[1974Dre]
IN-939	x(Al,Co,Cr,Ti,Ta,W) in γ and γ'	[1983Del]
Udimet-520	x(Al,Co,Cr,Ti,Mo,W) in γ and γ'	[1983Mag]
Udimet-710	x(Al,Co,Cr,Ti,Mo,W) in γ and γ'	[1983Mag]
Udimet-100	x(Al,Co,Cr,Ti,Mo,W) in γ and γ'	[1983Mag]
N-18	$T^{\gamma'}$	[1988Duc]
IN-100	$T^{\gamma'}$	[1988Duc]

Alloy	Experimental Information	References
MERL-76	$T^{\gamma'}$	[1988Duc]
RENE-95	$T^{\gamma'}$	[1988Duc]
ASTROLOY	$T^{\gamma'}$	[1988Duc]
Nimonic-105	x(Al,Co,Cr,Ti,Mo) in γ and γ'	[1991Tri]
BJH, BJJ, BJK, BJL, BJM, BJP	T^{l}, T^{s}, $T^{\gamma'}$	[1992Dha]
2D8625, 2D8638, 2D8639, 2D8640	T^{l}, T^{s}, $T^{\gamma'}$	[1992Dha]
MA6000	T^{l}, T^{s}, $T^{\gamma'}$	[1992Dha]
CMSX-2	T^{l}, T^{s}, $T^{\gamma'}$	[1992Dha]
SRR-99	x(Al,Co,Cr,Ti,Ta,W) in γ and γ'	[1992Sch]
Modified IN738LC	x(Al,Co,Cr,Mo,Ta,W) in γ and γ'	[1993Zha]
MC2	x(Al,Co,Cr,Mo,Ti,Ta,W) in γ and γ'	[1994Duv]
Ni-Al-Re-X(X: Cr, Mo, W, Ti, Ta, Nb, Co)	x(Al,RE, X) in γ and γ'	[1994Miy]
Rene N6	T^{l}, T^{s}, $T^{\gamma'}$, $f^{\gamma'}$ x(Al,Co,Cr,Mo,Ti,Ta,W) in γ and γ'	[1998Rit] [1999Rit] [2001Cop]

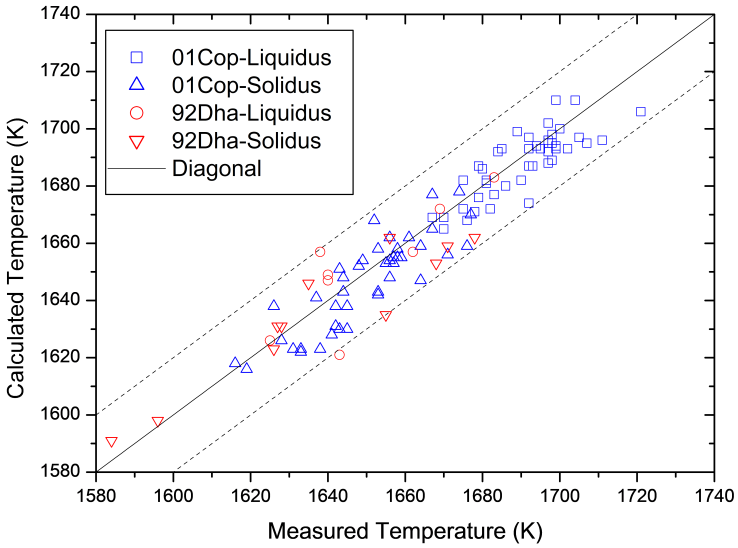


Figure 1.1: Comparison between the calculated and experimentally measured liquidus and solidus temperatures

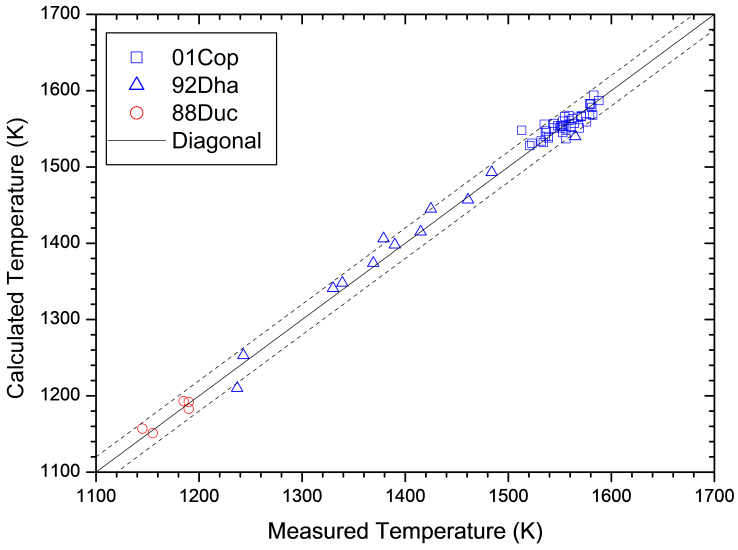


Figure 1.2: Comparison between the calculated and experimentally measured solvus temperatures of the γ' phase

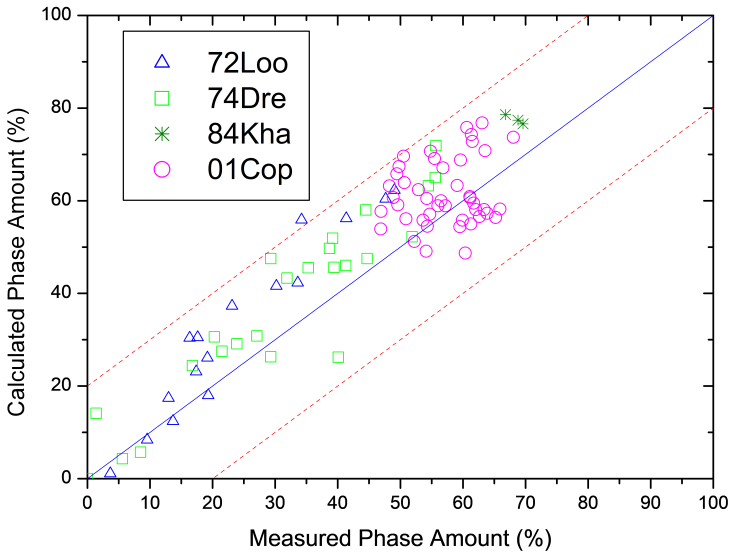


Figure 1.3: Comparison between the calculated and experimentally measured amounts of the γ' phase

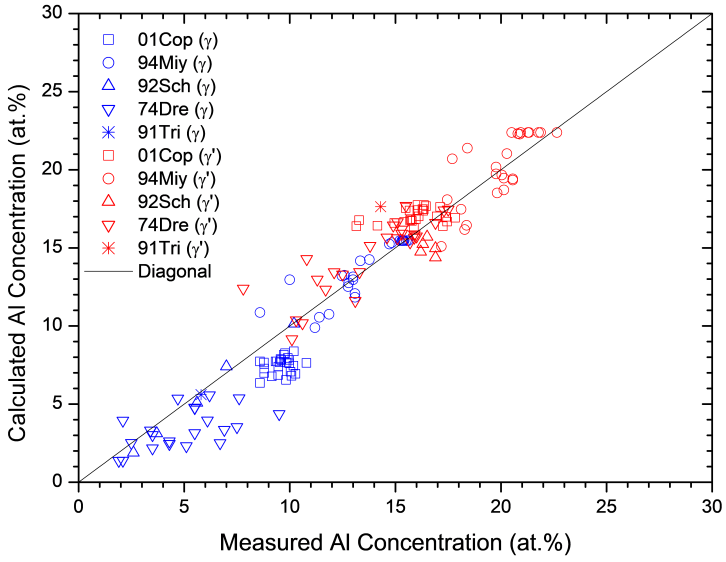


Figure 1.4: Comparison between the calculated and experimentally measured equilibrium compositions of Al in γ and γ' phase

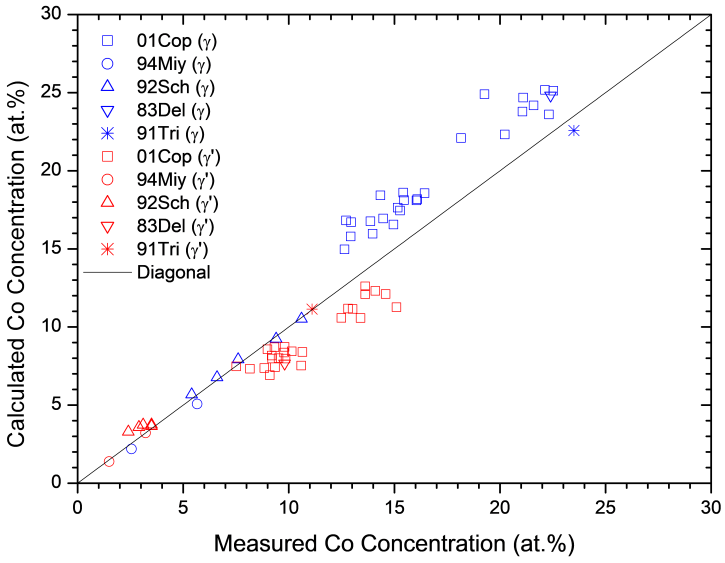


Figure 1.5: Comparison between the calculated and experimentally measured equilibrium compositions of Co in γ and γ' phases

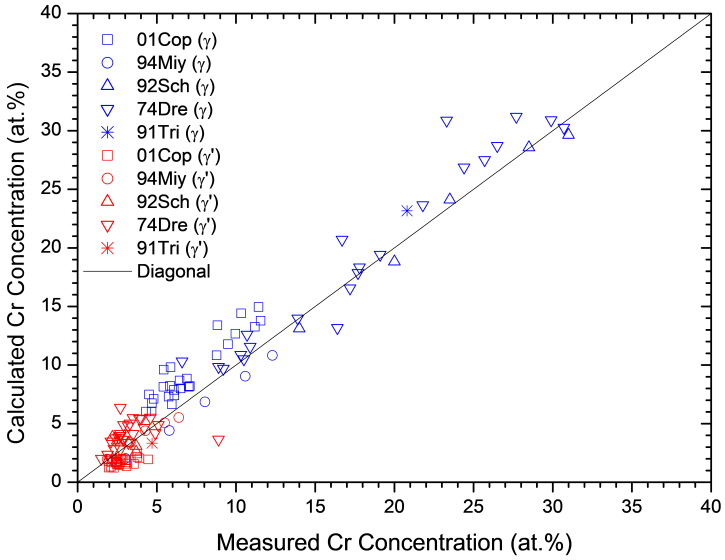


Figure 1.6: Comparison between the calculated and experimentally measured equilibrium compositions of Cr in γ and γ' phases

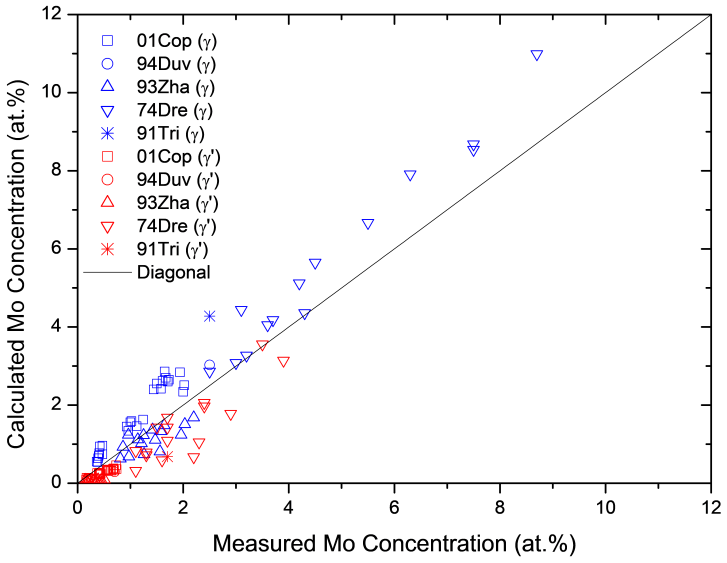


Figure 1.7: Comparison between the calculated and experimentally measured equilibrium compositions of Mo in γ and γ' phases

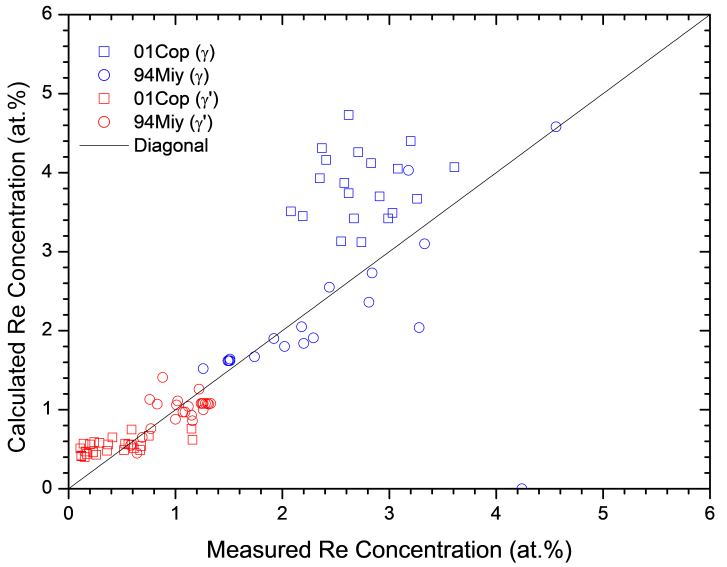


Figure 1.8: Comparison between the calculated and experimentally measured equilibrium compositions of Re in γ and γ' phases

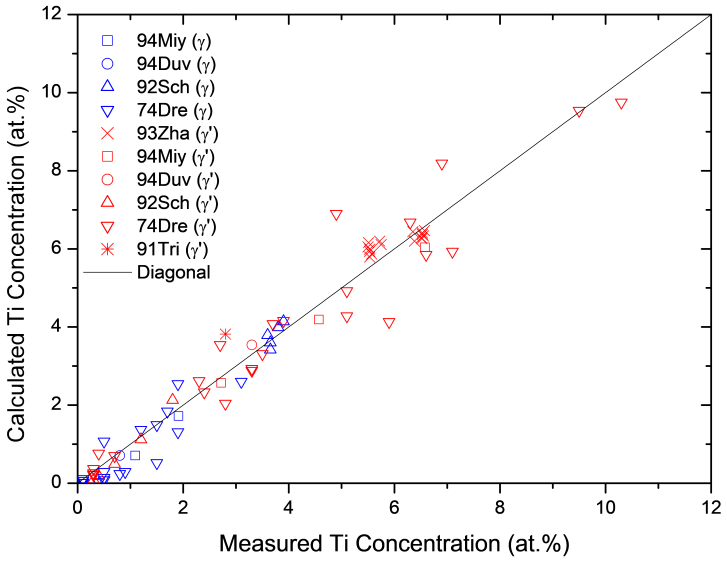


Figure 1.9: Comparison between the calculated and experimentally measured equilibrium compositions of Ti in γ and γ' phases

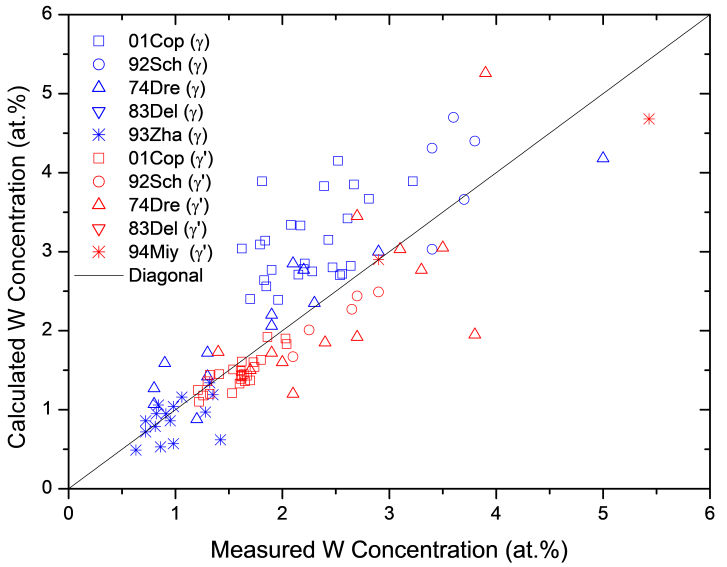


Figure 1.10: Comparison between the calculated and experimentally measured equilibrium compositions of W in γ and γ' phases

2 Mobility Database

PanNi2025_MB is an atomic mobility database for Ni-based alloys, which is compatible with the `PanNi2025_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	Hf	Ir	Mn	Mo	Nb	Ni	Pt	Re	Ru	Si	Ta	Ti	V	W	Y	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.

Fcc Phase

Al-Co	Al-Cu	Al-Mg	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-Ti	Cu-Zn	Fe-Mn	Fe-Ni
Fe-Si	Ir-Ni	Mn-Ni	Mo-Ni	Nb-Ni	Ni-Pt	Ni-Re	Ni-Ru	Ni-Ta	Ni-Ti
Ni-V	Ni-W	Ni-Zn							

Al-Co-W	Al-Cr-Ni	Al-Cu-Si	Al-Cu-Zn	Al-Mn-Ni	Al-Nb-Ni
Co-Cr-Ni	Co-Cr-W	Co-Cu-Fe	Co-Cu-Ni	Co-Fe-Ni	Co-Mo-W
Co-Ni-Re	Co-Ni-Ru	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	Hf-Zr	Mo-	Mo-Ta	Mo-Ti
Mo-W	Mo-Zr	Nb-Ta	Nb-Ti	Nb-W	Nb-Zr	Ta-Ti	Ta-W	Ti-Zr	

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

2.4 Database Validation

The simulated concentration profiles of a series of Ni-base alloys are shown below to validate the current `PanNi2025_MB` database.

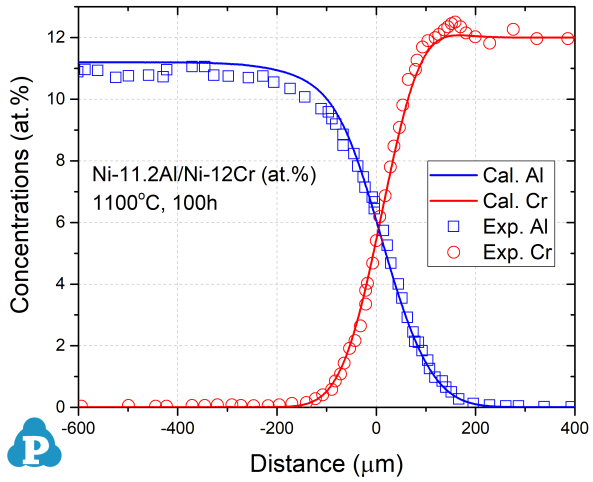


Figure 2.1: Concentration profiles of Ni-11.2Al/Ni-12Cr (at.%) at 1100 °C for 100h [1996Eng]

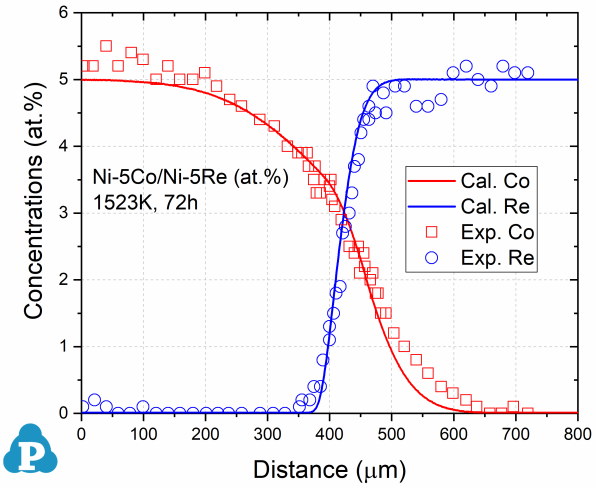


Figure 2.2: Concentration profiles of Ni-5Co/Ni-5Re (at.%) annealed at 1523K for 72h [2014Liu]

2.5 Applications

This mobility database is combined with the thermodynamic database for Ni-based superalloys, `PanNi2025_TH`, to simulate the diffusion-controlled phenomena of Ni-based superalloys. A few examples are given below.

Precipitation kinetics of Ni-based superalloys

The PanEvolution module was developed for the simulation of precipitation kinetics of multi-component alloys. It has been seamlessly integrated with the thermodynamic calculation engine of the Pandat software, and has been used to simulate the evolution of microstructure and the corresponding mechanical property responses to heat treatment of Ni-based superalloys. Below shows an example simulation performed for the LSHR alloy solutionized at supersolvus temperature 1463K for 20 minutes to dissolve γ' and homogenize the chemistry throughout the γ grain. These samples were then cooled at a rate of 11K/min or 139K/min to a predetermined temperature within the range of 1089K to 1411K, then quenched. The simulated γ' precipitates evolution is compared with experimental data as shown in Figure 2.3 and Figure 2.4. As is seen, the model calculated values agree well with those directly measured. The slow cooling rate leads to bimodal distribution of secondary γ' with much bigger particle size of secondary γ' (~3 times as big as the fast cooling rate) and slightly higher volume fraction of secondary γ'. The database used to do this simulation is the combined thermodynamic and mobility database of Ni-based alloys: `PanNi_TH+MB`. More information regarding to precipitation simulation can be found in **PanEvolution** module under the Software section.

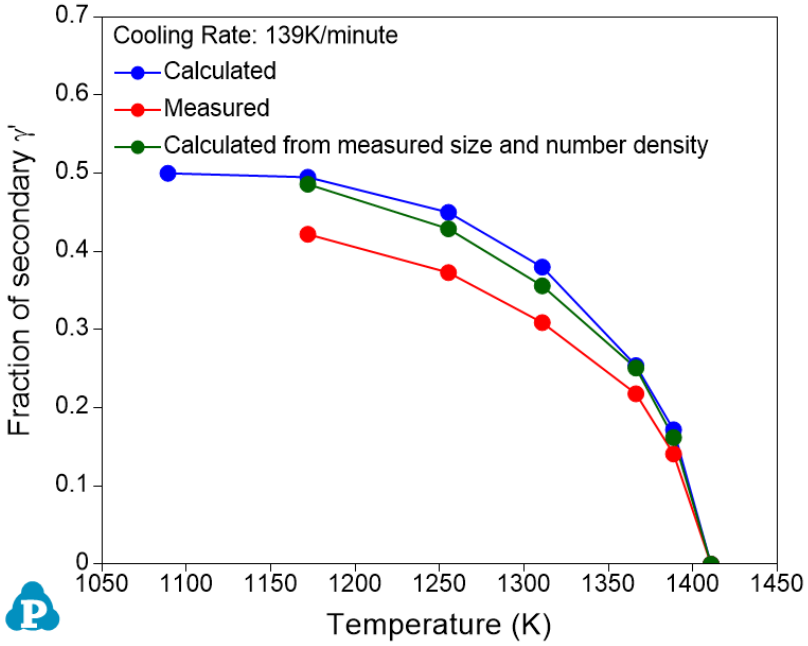


Figure 2.3: Comparison between the simulated and the measured volume fractions of γ' with the cooling speed of 139K/m to different temperatures

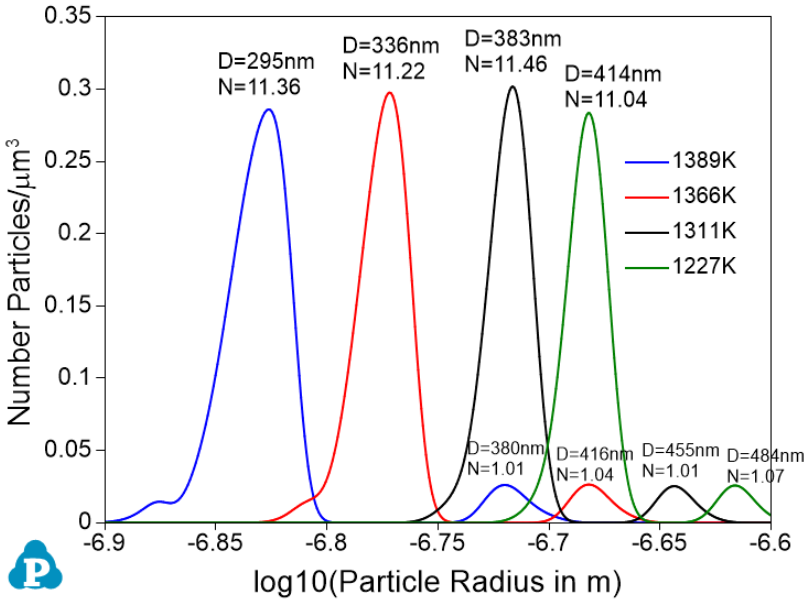


Figure 2.4: Simulated number densities of γ' particles when cooling to various temperatures with the cooling speed of 11K/m

Dissolution of Ni-based superalloys

The **PanDiffusion** module was developed for the simulation of diffusion kinetics of multi-component alloys. In Figure 2.5, dissolution of γ' particle in Ni-Al binary system was simulated for demonstration. The initial matrix composition is Ni-15at.%Al and that of the γ' particle is set as Ni-25at.%Al at the beginning with the radius of 5μm. The simulated composition profiles at 1200 °C for different time are shown in Figure 2.5. One can see that the γ' particle can be completed dissolved within a few minutes at 1200 °C. In this simulation, the combined thermodynamic and mobility database of Ni-based superalloys, `PanNi_TH+MB`, is used. More information regading to diffusion simulation can be found in **PanDiffusion** module under the Software section.

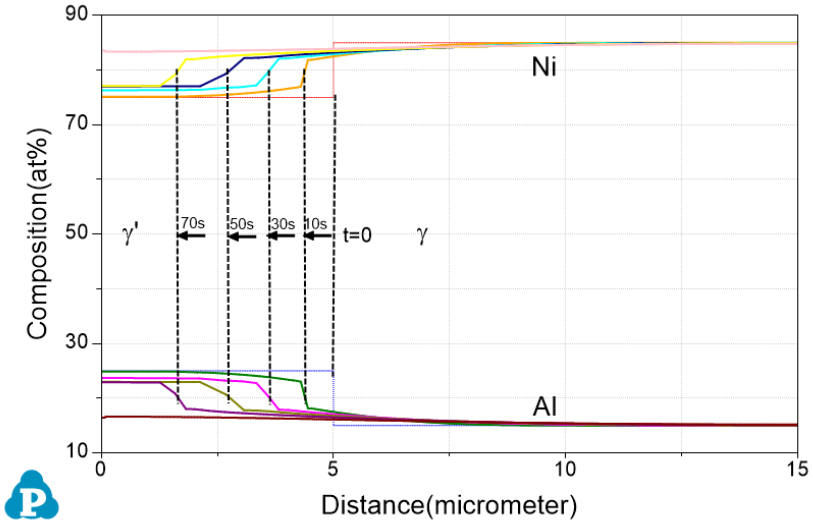


Figure 2.5: Simulated dissolution of γ' particle in Ni-Al binary system at 1200 °C

3 Thermophysical Property Database

The thermophysical property database **PanNi2025_TP**is compatible with the `PanNi2025_TH` thermodynamic database and suitable for the simulation of thermophysical properties of Ni-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 **343** phases assessed in the `PanNi2025_TH` database. It is used to calculate the density, thermal expansion, solidification shrinkage of Al alloys.

The simulated density changes vs. temperature of a series of Ni-based alloys are shown below to validate the current `PanNi2025_MV` database.

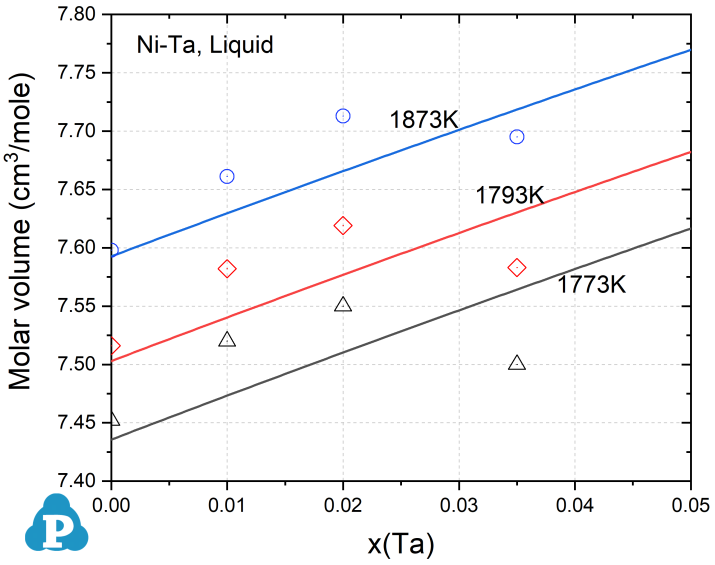


Figure 3.1: Molar volume of Ni-Ta liquid alloys [2004Muk, 2005Fan]

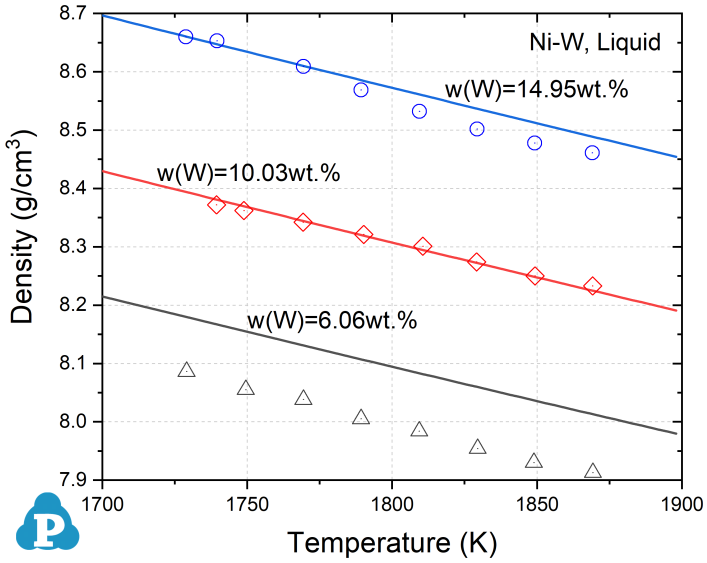


Figure 3.2: Density of Ni-W binary liquid mixture [2005Fan2]

3.2 Surface Tension

The surface tension of the liquid phase is added into the property database. Figure 3.3 shows the surface tension of a series of Al-Ni alloys in comparison with experimental data.

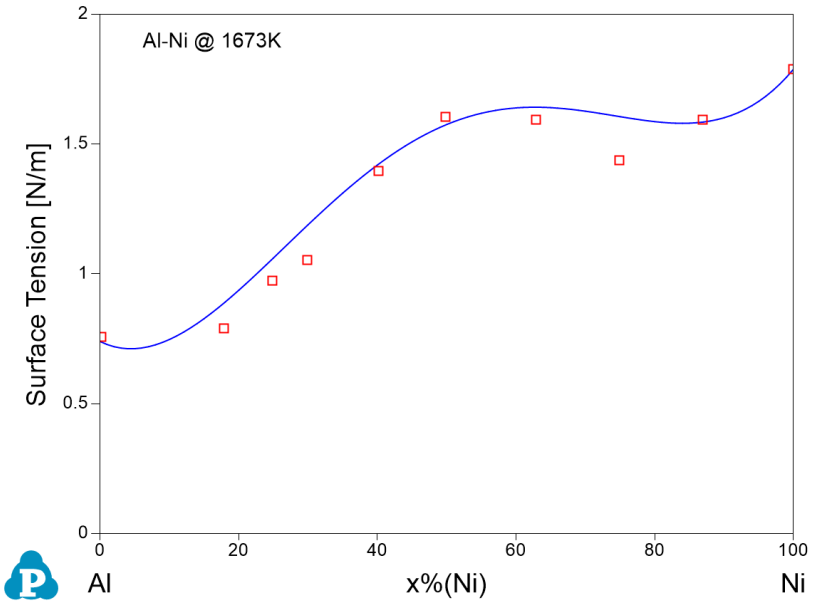


Figure 3.3: Surface tension of Al-Ni alloys

3.3 Viscosity

The viscosity of the liquid phase is added into the property database. Figure 3.4 shows the viscosity of Ni-Cr alloy in comparison with experimental data.

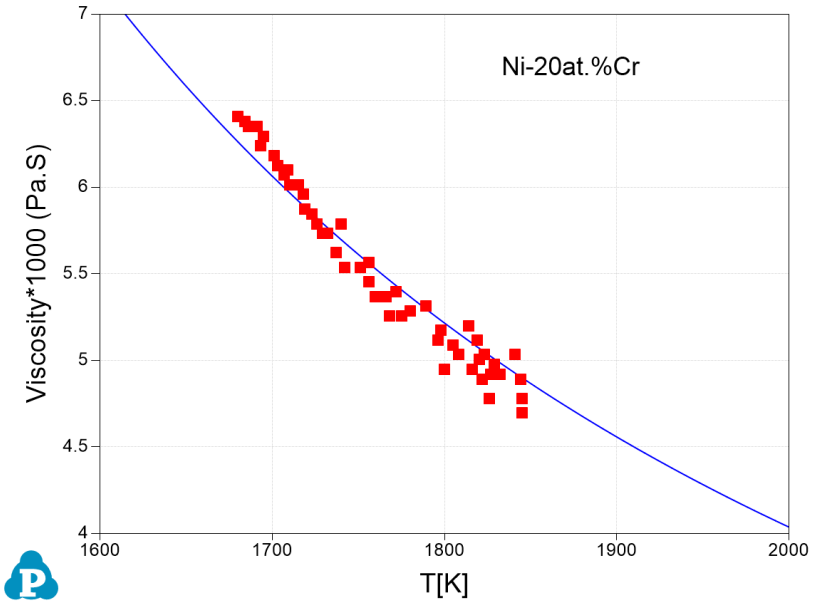


Figure 3.4: Viscosity of the Ni-Cr alloy

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PanNi2025: List of Phases

Phases (**343**)

Name	Model	Lattice Size	Constituent
A15	CEF (SLN)	(3)(1)	(Al,Cr,Fe,Ir,Mo,Nb,Pt,Ti,V) (Al,Co,Cr,Fe,Ir,Mo,Nb,Pt,Ti,V)
A2B_oS12	CEF (SLN)	(2)(1)	(Cu,Pt)(Ta,Ti)
A2B_tI6	CEF (SLN)	(2)(1)	(Co,Cr,Fe,Ni,Re,Ti,Zr)(Al,Cu,Ta)
A4B	CEF (SLN)	(4)(1)	(Ni)(Mo,W)
A8B	CEF (SLN)	(8)(1)	(Fe,Ni)(Nb,Ta)
AB2_oI6	CEF (SLN)	(1)(2)	(Al,Cr,Mo,Pt,V)(Mo,Ni,Pt)
AB2_tI12	CEF (SLN)	(1)(2)	(Al,Co,Cr,Fe,Ni) (Hf,Nb,Ta,Ti,V,W,Zr)
AB3_oP16	CEF (SLN)	(1)(3)	(Co,Ni)(Al,Y)
AB_oS8	CEF (SLN)	(1)(1)	(Al,Co,Ni)(Hf,W,Y,Zr)
A_TiO	CEF (ST2)	(1)(1)	(Ti)(O)
Al10V	CEF (ST2)	(10)(1)	(Al)(V)
Al11Cr2	CEF (ST2)	(10)(1)(2)	(Al)(Al)(Cr)
Al11M4	CEF (SLN)	(11)(4)	(Al)(Mn,Re)
Al11Mn4_HT	CEF (SLN)	(29)(10)	(Al,Mn)(Mn)
Al12M	CEF (SLN)	(12)(1)	(Al)(Mn,Re)
Al13Co4	CEF (ST2)	(13)(4)	(Al)(Co)
Al13Cr2	CEF (ST2)	(13)(2)	(Al)(Cr)
Al13Ir4	CEF (ST2)	(0.765) (0.235)	(Al)(Ir)

Name	Model	Lattice Size	Constituent
Al13Ru4	CEF (SLN)	(0.6275) (0.235) (0.1375)	(Al)(Ni,Ru)(Al,Va)
Al14Ni2Ru	CEF (SLN)	(0.94118) (0.05882)	(Al,Ni)(Ru)
Al1Fe1O3	CEF (ST3)	(1)(1)(3)	(Al+3)(Fe+3)(O-2)
Al21Pt5	CEF (ST2)	(0.807692) (0.192308)	(Al)(Pt)
Al21Pt8	CEF (ST2)	(0.724138) (0.275862)	(Al)(Pt)
Al23V4	CEF (ST2)	(23)(4)	(Al)(V)
Al2Hf3	CEF (ST2)	(2)(3)	(Al)(Hf)
Al2Pt	CEF (SLN)	(0.666667) (0.333333)	(Al)(Ni,Pt)
Al2Ru	CEF (SLN)	(2)(1)(1)	(Al)(Ru)(Al,Ru,Va)
Al2S3	CEF (ST2)	(2)(3)	(Al)(S)
Al2Y3	CEF (ST2)	(0.4)(0.6)	(Al)(Y)
Al3Co	CEF (ST2)	(3)(1)	(Al)(Co)
Al3Hf2	CEF (ST2)	(3)(2)	(Al)(Hf)
Al3Hf4	CEF (ST2)	(3)(4)	(Al)(Hf)
Al3Hf_Alpha	CEF (ST2)	(3)(1)	(Al)(Hf)
Al3Hf_Beta	CEF (ST2)	(3)(1)	(Al)(Hf)
Al3Ir	CEF (ST2)	(0.75)(0.25)	(Al)(Ir)
Al3M2	CEF (SLN)	(3)(2)(1)	(Al)(Al,Ni,Pt,Ru,V)(Ru,Ni,Pt,Va)
Al3Ni5	CEF (ST2)	(0.375)	(Al)(Ni)

Name	Model	Lattice Size	Constituent
		(0.625)	
Al3Pt5	CEF (SLN)	(0.375) (0.625)	(Al)(Ni,Pt)
Al45Ir13	CEF (ST2)	(0.776) (0.224)	(Al)(Ir)
Al4M	CEF (SLN)	(4)(1)	(Al)(Cr,Mo,W)
Al4Mn	CEF (ST2)	(4)(1)	(Al)(Mn)
Al4Mn_L	CEF (ST2)	(461)(107)	(Al)(Mn)
Al4Re	CEF (ST2)	(4)(1)	(Al)(Re)
Al5Co2	CEF (SLN)	(5)(2)	(Al)(Co,Fe)
Al69Ta39	CEF (SLN)	(0.6389) (0.3611)	(Al,Ta)(Al,Ta)
Al6M	CEF (SLN)	(6)(1)	(Al)(Mn,Ru,Re)
Al73Ir27	CEF (ST2)	(0.73)(0.27)	(Al)(Ir)
Al7V	CEF (ST2)	(7)(1)	(Al)(V)
Al8Cr5_H	CEF (ST2)	(8)(5)	(Al)(Cr)
Al8Cr5_L	CEF (ST2)	(8)(5)	(Al)(Cr)
Al8Mn5	CEF (SLN)	(12)(5)(9)	(Al)(Mn)(Al,Mn)
Al8V5	CEF (SLN)	(8)(5)	(Al)(Ni,V)
Al9Co2	CEF (ST2)	(9)(2)	(Al)(Co)
Al9Cr4_H	CEF (ST2)	(9)(4)	(Al)(Cr)
Al9Cr4_L	CEF (ST2)	(9)(4)	(Al)(Cr)
Al9Ir2	CEF (ST2)	(0.818) (0.182)	(Al)(Ir)
AlNi8Y3	CEF (ST3)	(1)(8)(3)	(Al)(Ni)(Y)

Name	Model	Lattice Size	Constituent
AlPt	CEF (SLN)	(0.5)(0.5)	(Al)(Ni,Pt)
AlRe	CEF (ST2)	(1)(1)	(Al)(Re)
AlS	CEF (ST2)	(1)(1)	(Al)(S)
AlY	CEF (ST2)	(0.5)(0.5)	(Al)(Y)
AlY2	CEF (ST2)	(0.333333) (0.666667)	(Al)(Y)
Alpha	CEF (SLN)	(0.5)(0.25) (0.25)	(Al,Ni,Pt)(Al,Ni,Pt)(Al,Ni,Pt)
Alpha_B	CEF (ST1)	(1)	(B)
Alpha_M5Si3	CEF (SLN)	(5)(3)	(Nb,Ta,W)(Si)
Alpha_TiMn	CEF (ST2)	(1)(1)	(Mn)(Ti)
B19	CEF (SLN)	(0.5)(0.5)	(Mo,Pt,V)(Mo,Pt,V)
B2	CEF (SLN)	(1)(1)	(Al,Co,Cr,Fe,Hf,Ir,Mn,Mo,Nb,Ni, Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr) (Al,Co,Cr,Cu,Fe,Hf,Ir,Mn,Mo,Nb, Ni,Pt,Re,Ru,Si,Ta,Ti,V,W,Va)
B2O3	CEF (ST2)	(2)(3)	(B)(O)
BCC_A12	CEF (SLN)	(1)(1)	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Pt,Si, Ta,Ti,V)(Va)
BETA_VO	CEF (SLN)	(1)(1)	(V)(O,Va)
Bcc	CEF (SLN)	(1)(3)	(Al,Co,Cr,Cu,Fe,Hf,Ir,Mn,Mo,Nb, Ni,P,Pt,Re,Ru,S,Si,Ta,Ti,V, W,Y,Zr) (B,C,N,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)

Name	Model	Lattice Size	Constituent
Beta2_Ni3Si	CEF (SLN)	(3)(1)	(Ni)(Si,Ti)
Beta_B	CEF (ST1)	(93)(12)	(B)(B)
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_TiMn	CEF (ST2)	(0.515) (0.485)	(Mn)(Ti)
CUB_A13	CEF (SLN)	(1)(1)	(Al,Co,Cu,Cr,Fe,Hf,Mn,Mo,Nb, Ni,Pt,Si,Ta,Ti,V)(Va)
Chi_A12	CEF (SLN)	(24)(10)(24)	(Cr,Fe,Ni,Re)(Cr,Mo,Ta,W) (Cr,Fe,Mo,Ni,Re,Ta,W)
Co11Zr2	CEF (ST2)	(11)(2)	(Co)(Zr)
Co17Y2	CEF (SLN)	(17)(2)	(Co,Ni)(Y)
Co2P	CEF (ST2)	(2)(1)	(Co)(P)
Co3M	CEF (SLN)	(3)(1)	(Co)(V,Y)
Co3Si	CEF (ST2)	(0.75)(0.25)	(Co)(Si)
Co3Y2	CEF (ST2)	(3)(2)	(Co)(Y)
Co3Y4	CEF (ST2)	(3)(4)	(Co)(Y)
Co5Y8	CEF (ST2)	(5)(8)	(Co)(Y)
Co7Ta2	CEF (ST2)	(7)(2)	(Co)(Ta)
Co7Y6	CEF (ST2)	(7)(6)	(Co)(Y)
CoZr3	CEF (ST2)	(1)(3)	(Co)(Zr)
Corundum	CEF (SLN)	(2)(1)(3)	(Al+3,Cr+2,Cr+3,Fe+2,Fe+3,Ti+3, V+3,V+4,Va)(Cr+3,Fe+3,Ni+2,Va) (O-2)
Cr2B	CEF (ST2)	(0.667)	(Cr)(B)

Name	Model	Lattice Size	Constituent
		(0.333)	
Cr3Mn5	CEF (ST2)	(3)(5)	(Cr)(Mn)
Cr3Ru	CEF (ST2)	(0.685) (0.315)	(Cr)(Ru)
Cr5B3	CEF (ST2)	(0.625) (0.375)	(Cr)(B)
CrB	CEF (SLN)	(0.5)(0.5)	(Cr,Ni,V)(B)
CrB4	CEF (ST2)	(0.2)(0.8)	(Cr)(B)
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)
Cu2Y_H	CEF (ST2)	(2)(1)	(Cu)(Y)
Cu2Y_R	CEF (ST2)	(2)(1)	(Cu)(Y)
Cu33Si7	CEF (ST2)	(0.825) (0.175)	(Cu)(Si)
Cu3P	CEF (ST2)	(3)(1)	(Cu)(P)
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)
Cu4Y	CEF (ST2)	(4)(1)	(Cu)(Y)
Cu6Y	CEF (SLN)	(5)(1)	(Cu)(Cu2,Y)
Cu7Y2	CEF (ST2)	(7)(2)	(Cu)(Y)

Name	Model	Lattice Size	Constituent
CuO	CEF (ST2)	(1)(1)	(Cu)(O)
CuTi	CEF (SLN)	(0.5)(0.5)	(Cu,Ti)(Cu,Ti)
D0_19	CEF (SLN)	(0.75)(0.25) (0.5)	(Al,Co,Cr,Mn,Mo,Nb,Ni,Pt,Ta,Ti,V,Zr) (Al,Co,Cr,Mn,Mo,Nb,Pt,Si,Ta,Ti,W,Zr)(Va)
D0_22	CEF (SLN)	(0.75)(0.25) (0.5)	(Al,Cr,Mo,Ni,Pt,Si,Ti)(Al,Cr,Mo,Nb, Pt,Ta,Ti,V)(C,Va)
Delta	CEF (SLN)	(3)(1)	(Al,Co,Cr,Fe,Nb,Ni,Re,Ta,Ti) (Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Si,Ta,Ti,W,Zr)
Diamond_Si	CEF (SLN)	(1)	(C,Si)
Epsilon_Ni3Si2	CEF (SLN)	(3)(2)	(Co,Fe,Ni)(Si)
Eta	CEF (SLN)	(0.75)(0.25)	(Co,Cu,Fe,Ni,Ti) (Al,Cr,Hf,Mo,Nb,Ni,Si,Ta,Ti,V,Zr)
Fcc	CEF (SLN)	(1)(1)	(Al,Co,Cr,Cu,Fe,Hf,Ir,Mn,Mo,Nb,Ni, P,Pt,Re,Ru,S,Si,Ta,Ti,V,W,Y,Zr) (B,C,N,O,Va)
Fcc_MC	CEF (SLN)	(1)(1)	(Co,Cr,Fe,Hf,Mo,Nb,Ni,Si,Ta,Ti,V, W,Zr) (B,C,N,Va)
Fe3Si7	CEF (ST2)	(0.3)(0.7)	(Fe)(Si)
Fe4Re	CEF (SLN)	(4)(1)	(Fe,Re)(Fe,Re)
FeB	CEF (ST2)	(1)(1)	(Fe)(B)
FeNb2P	CEF (ST3)	(1)(2)(1)	(Fe)(Nb)(P)
FeNb4P	CEF (ST3)	(1)(4)(1)	(Fe)(Nb)(P)
FeNbP	CEF (SLN)	(2)(1)	(Fe,Nb)(P)
FeP2	CEF (ST2)	(1)(2)	(Fe)(P)
FeP4	CEF (ST2)	(1)(4)	(Fe)(P)

Name	Model	Lattice Size	Constituent
FeS	CEF (SLN)	(1)(1)	(Cr,Fe,Mn,Ni,Ti,Va)(S)
FeS2	CEF (SLN)	(1)(2)	(Fe,Mn)(S)
FeTiP	CEF (SLN)	(1)(2)(1)	(Fe,Ti)(Fe,Ti)(P)
GAS	GAS	(1)	(Al,AlO,AlO2,Al2,Al2O,Al2O2,Al2O3, C1O1,C1O2,Fe,FeO,FeO2,Fe2, Hf,HfO,HfO2,Ir,IrO2,IrO3,Mn,O,O2, O3,P,PO,PO2,P4O6,P4O10, S,S2,S3,S4,S5,S6,S7,S8,S2O, SO,SO2,SO3,Si,Si2,Si3,SiO,SiO2, Ti,TiO,TiO2,Y,YO,Zr,Zr2,ZrO,ZrO2)
Gamma_ Ni5Si2	CEF (SLN)	(5)(2)	(Co,Cr,Fe,Ni)(Al,Si)
Gamma_ double_prime	CEF (SLN)	(3)(1)	(Al,Co,Cr,Fe,Nb,Ni,Re,Ta,Ti) (Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Ta,Ti,W)
Graphite	CEF (ST1)	(1)	(C)
Halite	CEF (SLN)	(1)(1)	(Al+3,Co+2,Cr+3,Fe+2,Fe+3, Mn+2,Mn+3,Ni+2,V,V+2,V+3,Va)(O-2,Va)
Hcp	CEF (SLN)	(1)(0.5)	(Al,Co,Cr,Cu,Fe,Hf,Ir,Mn,Mo, Nb,Ni,Pt,Re,Ru,S,Si,Ta,Ti, V,W,Y,Zr) (B,C,N,O,Va)
Hcp_M2C	CEF (SLN)	(1)(0.5)	(Co,Cr,Fe,Mo,Nb,Ni,Ta,Ti,V,W) (B,C,N,Va)
HfMn	CEF (ST2)	(0.5)(0.5)	(Hf)(Mn)
HfSiO4	CEF (ST3)	(1)(1)(4)	(Hf)(Si)(O)
Ir2Y3	CEF (ST2)	(2)(3)	(Ir)(Y)
Ir2Y5	CEF (ST2)	(2)(5)	(Ir)(Y)
Ir3Y5	CEF (ST2)	(3)(5)	(Ir)(Y)

Name	Model	Lattice Size	Constituent
IrY3	CEF (ST2)	(1)(3)	(Ir)(Y)
L10	CEF (SLN)	(1)(1)	(Al,Mn,Ni,Pt,Ti)(Al,Mn,Ni,Pt,Ti)
L12_FCC	CEF (SLN)	(0.75)(0.25)(1)	(Al,Co,Cr,Fe,Hf,Ir,Mn,Mo,Nb,Ni,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr)(Al,Co,Cr,Fe,Hf,Ir,Mn,Mo,Nb,Ni,Pt,Re,Ru,Si,Ta,Ti,V,W,Y,Zr)(Va)
L_Sigma_CrMn	CEF (SLN)	(8)(4)(18)	(Mn)(Cr)(Cr,Mn)
Laves_C14	CEF (SLN)	(2)(1)	(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Re,Ru,Si,Ta,Ti,V,W,Zr)(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Ta,Ti,W,Y,Zr)
Laves_C15	CEF (SLN)	(2)(1)	(Al,Co,Cr,Fe,Hf,Ir,Mn,Mo,Nb,Ni,Ru,Ta,Ti,V,W,Y,Zr)(Al,Co,Cr,Fe,Hf,Ir,Mo,Nb,Ni,Ta,Ti,W,Y,Zr)
Laves_C36	CEF (SLN)	(2)(1)	(Co,Cr,Ta,Ti)(Co,Cr,Ta,Ti)
Liquid	CEF (SLN)	(1)	(Al,B,C,Co,Cr,Cu,Fe,Hf,Ir,Mn,Mo,N,Nb,Ni,O,P,Pt,Re,Ru,S,Si,Ta,Ti,V,W,Y,Zr,Co2P,Cu3P,Al2S3,Cr1S1,Fe1S1,Mo2S3,Ni1S1,Mn1S1,Al2O3,B2O3,CoO,Co2O3,Cr2/3O,CuO,Cu2O,Cu2O3,FeO,FeO3/2,HfO2,MnO,Mn2/3O,MoO2,MoO3,NbO,NbO2,Nb2O5,NiO,P,P4O10,P4O6,SO3,SiO2,Ta2O5,TiO,TiO3/2,TiO2,VO,VO2,VO3/2,VO5/2,WO2,WO3,Y2O3,Zr1/2O)
M17Y2	CEF (SLN)	(17)(2)	(Al,Co,Cu,Fe,Ni,Ru)(Y)

Name	Model	Lattice Size	Constituent
M23C6	CEF (SLN)	(20)(3)(6)	(Co,Cr,Fe,Ni,Re) (Co,Cr,Fe,Mo,Nb,Ni,Re,Ta,Ti,W) (B,C)
M23N6	CEF (SLN)	(23)(6)	(Co,Fe,Mn)(Y,Zr)
M2B	CEF (SLN)	(2)(1)	(Co,Cr,Fe,Mo,Ni,Ta,W)(B)
M2P	CEF (SLN)	(2)(1)	(Cr,Fe,Mn,Mo,Nb,Ni,Ti)(P)
M2Si_oP12	CEF (SLN)	(2)(1)	(Co,Cr,Fe,Ni,Ru,Si)(Al,Co,Si)
M2Si_tI12	CEF (SLN)	(2)(1)	(Hf,Ta,Zr)(Si)
M3B2	CEF (SLN)	(2)(1)(2)	(Co,Cr,Fe,Mo,Nb,Ni,Ta,V,W) (Co,Cr,Fe,Nb,Ni,Ta,V,W)(B)
M3BC	CEF (SLN)	(3)(1)	(Co,Cr,Fe,Ni)(B,C)
M3C2	CEF (SLN)	(3)(2)	(Cr,Mo,V,W)(C)
M3P	CEF (SLN)	(3)(1)	(Cr,Fe,Mn,Mo,Ni,Ti)(P)
M3Si2	CEF (SLN)	(2)(3)	(Si)(Hf,Zr)
M3Si_cF16	CEF (SLN)	(3)(1)	(Mn,Ni)(Al,Si,Ti)
M3Si_cP8	CEF (SLN)	(3)(1)(3)	(Cr,Mo,Nb,Ni,Si,V)(Cr,Mo,Si,V)(Va)
M3Si_tP32	CEF (SLN)	(3)(1)	(Mo,Nb,Ta,Ti,Zr)(Si)
M3Y	CEF (SLN)	(3)(1)	(Al,Fe,Ni,Ir,Ru)(Y)
M4C3	CEF (ST2)	(4)(3)	(Al)(C)
M5Si3	CEF (SLN)	(0.5)(0.125) (0.375)	(Cr,Mo,Nb,Ta,Ti,V,W,Zr) (Cr,Mo,Nb,Si,Ta,Ti,V,W,Zr) (Mo,Nb,Si)
M5Si4	CEF (SLN)	(5)(4)	(Hf,Ti,Zr)(Si)
M5Y	CEF (SLN)	(5)(1)	(Co,Cu,Fe,Ni,Ru,Si)(Y)
M6C	CEF (SLN)	(2)(2)(2)(1)	(Co,Fe,Ni)(Cr,Mo,Nb,W) (Co,Cr,Fe,Mo,Nb,Ni,W)(C)
M7C3	CEF (SLN)	(7)(3)	(Co,Cr,Fe,Mo,Nb,Ni,Re,W)(B,C)

Name	Model	Lattice Size	Constituent
M7Y2	CEF (SLN)	(7)(2)	(Co,Fe,Ni,Ru)(Y)
MB2	CEF (SLN)	(1)(2)	(Al,Cr,Hf,Mo,Nb,Re,Ta,Ti,V,Zr)(B)
MO2	CEF (SLN)	(1)(2)	(Hf,Mo,V,W,Zr)(O)
MP	CEF (SLN)	(1)(1)	(Co,Cr,Fe,Mn)(P)
MSi2_cF12	CEF (SLN)	(1)(2)	(Co,Fe,Mn,Ni)(Al,Si)
MSi2_hP9	CEF (SLN)	(1)(2)	(Cr,Mo,Nb,Si,Ta,V)(Cr,Si)
MSi2_oC12	CEF (SLN)	(2)(1)	(Si)(Hf,Zr)
MSi2_oC48	CEF (SLN)	(1)(2)	(Fe,Ni)(Si)
MSi2_tI6	CEF (SLN)	(1)(2)	(Mo,Nb,Re,W)(Si,Va)
MSi_cP8	CEF (SLN)	(1)(1)	(Co,Cr,Fe,Mn,Nb,Ni,Re,Ru,Si,Ti,Zr) (Al,Co,Si)
MSi_oC8	CEF (SLN)	(1)(1)	(Si)(Y,Zr)
MSi_oP8	CEF (SLN)	(1)(1)	(Co,Fe,Hf,Ni,Pt,Ti,Zr)(Al,Si)
Mn11Si19	CEF (ST2)	(11)(19)	(Mn)(Si)
Mn12Y	CEF (ST2)	(12)(1)	(Mn)(Y)
Mn3O4_A	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3O4_B	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3P2	CEF (ST2)	(3)(2)	(Mn)(P)
Mn3Ti	CEF (ST2)	(3)(1)	(Mn)(Ti)
Mn4Ti	CEF (ST2)	(0.815) (0.185)	(Mn)(Ti)
Mn5Si3	CEF (SLN)	(2)(3)(3)(1)	(Fe,Hf,Mn,Ni,Si,Ti,Y,Zr)(Ni,Si,Ti) (Fe,Hf,Mn,Ti,Y,Zr)(Va)
Mn6Si	CEF (ST2)	(17)(3)	(Mn)(Si)
Mn9Si2	CEF (ST2)	(33)(7)	(Mn)(Si)

Name	Model	Lattice Size	Constituent
MnNi2	CEF (SLN)	(1)(2)	(Mn,Ni)(Ni)
MnP4	CEF (ST2)	(1)(4)	(Mn)(P)
MnPt7	CEF (ST2)	(1)(7)	(Mn)(Pt)
MnS	CEF (SLN)	(1)(1)	(Cr,Fe,Mn)(S)
Mo2S3	CEF (ST2)	(2)(3)	(Mo)(S)
Mo3P	CEF (ST2)	(3)(1)	(Mo)(P)
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)
MoO3	CEF (ST2)	(1)(3)	(Mo)(O)
MoP	CEF (ST2)	(1)(1)	(Mo)(P)
MoS2	CEF (ST2)	(1)(2)	(Mo)(S)
Mu_Phase	CEF (SLN)	(7)(2)(4)	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Re,Ta,W) (Co,Cr,Mo,Nb,Ni,Re,Ta,Ti,W) (Co,Cr,Fe,Mo,Nb,Ni,Re,Ta,Ti,W)
Nb2O5	CEF (ST2)	(2)(5)	(Nb)(O)
Nb3P	CEF (ST2)	(3)(1)	(Nb)(P)
Nb7P4	CEF (ST2)	(7)(4)	(Nb)(P)
NbO	CEF (ST2)	(1)(1)	(Nb)(O)
NbO2	CEF (ST2)	(1)(2)	(Nb)(O)
NbP	CEF (ST2)	(1)(1)	(Nb)(P)
NbP2	CEF (ST2)	(1)(2)	(Nb)(P)

Name	Model	Lattice Size	Constituent
Ni10Hf7	CEF (SLN)	(10)(7)	(Ni)(Hf,Ti,Zr)
Ni11Hf9	CEF (SLN)	(11)(9)	(Ni)(Hf,Zr)
Ni12P5_H	CEF (ST2)	(12)(5)	(Ni)(P)
Ni12P5_L	CEF (ST2)	(12)(5)	(Ni)(P)
Ni16Si7Ti6	CEF (SLN)	(16)(7)(6)	(Ni)(Si)(Nb,Si,Ti)
Ni21Hf8	CEF (SLN)	(21)(8)	(Ni)(Hf,Zr)
Ni2Y3	CEF (ST2)	(2)(3)	(Ni)(Y)
Ni3Hf_Alpha	CEF (SLN)	(3)(1)	(Ni)(Hf,Ti)
Ni3Hf_Beta	CEF (ST2)	(3)(1)	(Ni)(Hf)
Ni3S2	CEF (ST2)	(0.6)(0.4)	(Ni)(S)
Ni4Y	CEF (ST2)	(4)(1)	(Ni)(Y)
Ni5Hf	CEF (SLN)	(5)(1)	(Ni)(Hf,Zr)
Ni5P2_H	CEF (ST2)	(5)(2)	(Ni)(P)
Ni5P2_L	CEF (ST2)	(5)(2)	(Ni)(P)
Ni5P4	CEF (ST2)	(5)(4)	(Ni)(P)
Ni6AlTa	CEF (ST3)	(6)(1)(1)	(Ni)(Al)(Ta)
Ni7Hf2	CEF (SLN)	(7)(2)	(Al,Cr,Ni)(Hf,Ni,Ti,Zr)
Ni7Hf3	CEF (ST2)	(7)(3)	(Ni)(Hf)
NiHf_Beta	CEF (ST2)	(1)(1)	(Ni)(Hf)
NiMo	CEF (SLN)	(24)(20)(12)	(Co,Cr,Fe,Ni) (Al,Cr,Fe,Mo,Ni,Re,W)(Mo)
NiP2	CEF (SLN)	(1)(2)	(Cr,Ni)(P)
NiS2	CEF (ST2)	(1)(2)	(Ni)(S)
NiTiZr	CEF (SLN)	(1)(1)(1)	(Ni,Ti,Zr)(Ni,Ti,Zr)(Ni,Ti,Zr)
NiV3	CEF (ST2)	(0.25)(0.75)	(Ni)(V)

Name	Model	Lattice Size	Constituent
NiY	CEF (SLN)	(1)(1)	(Co,Ni)(Y)
Orthorhombic	CEF (ST1)	(1)	(S)
P4O10	CEF (ST2)	(4)(10)	(P)(O)
P_Phase	CEF (SLN)	(24)(12)(20)	(Co,Cr,Fe,Ni,Re)(Mo,W) (Co,Cr,Fe,Mo,Ni,Re,W)
P_Red	CEF (ST1)	(1)	(P)
P_White	CEF (ST1)	(1)	(P)
Phi	CEF (SLN)	(0.8837) (1.1163)	(Al,Ta)(Al,Ta)
Pt2Si_beta	CEF (ST2)	(0.667) (0.333)	(Pt)(Si)
PtO2	CEF (ST2)	(1)(2)	(Pt)(O)
PtTa	CEF (ST2)	(1)(1)	(Pt)(Ta)
PtTa6	CEF (ST2)	(1)(6)	(Pt)(Ta)
Quartz	CEF (ST2)	(1)(2)	(Si)(O)
R_Phase	CEF (SLN)	(27)(14)(12)	(Co,Cr,Fe,Mo,Ni)(Mo,W) (Co,Cr,Fe,Mo,Ni,W)
Re24Zr5	CEF (ST2)	(0.8276) (0.1724)	(Re)(Zr)
Re25Zr21	CEF (ST2)	(0.5435) (0.4565)	(Re)(Zr)
Re2O7	CEF (ST2)	(2)(7)	(Re)(O)
Re2Si	CEF (ST2)	(2)(1)	(Re)(Si)
ReO2	CEF (ST2)	(1)(2)	(Re)(O)
ReO3	CEF (ST2)	(1)(3)	(Re)(O)

Name	Model	Lattice Size	Constituent
Ru25Y44	CEF (ST2)	(0.362) (0.638)	(Ru)(Y)
Ru2Si3	CEF (ST2)	(0.4)(0.6)	(Ru)(Si)
Ru2Y3	CEF (ST2)	(0.4)(0.6)	(Ru)(Y)
Ru2Y5	CEF (ST2)	(0.286) (0.714)	(Ru)(Y)
Ru4Si3	CEF (ST2)	(0.5714) (0.4286)	(Ru)(Si)
Ru5Ta3	CEF (ST2)	(0.625) (0.375)	(Ru)(Ta)
RuY3	CEF (ST2)	(0.25)(0.75)	(Ru)(Y)
Rutile	CEF (SLN)	(1)(2)	(Ir+4,Mn+4,Ru+4,Ti+3,Ti+4,V+4)(O-2,Va)
Shp_MC	CEF (SLN)	(1)(1)	(Mo,W)(C,N)
Si2Y_H	CEF (ST2)	(2)(1)	(Si)(Y)
Si2Y_R	CEF (ST2)	(2)(1)	(Si)(Y)
Si4Y5	CEF (ST2)	(4)(5)	(Si)(Y)
Si5V6	CEF (ST2)	(0.454545) (0.545455)	(Si)(V)
Si5Y3_H	CEF (ST2)	(5)(3)	(Si)(Y)
Si5Y3_R	CEF (ST2)	(5)(3)	(Si)(Y)
SiO_AM	CEF (ST2)	(1)(1)	(Si)(O)
Sigma	CEF (SLN)	(8)(4)(18)	(Al,Co,Fe,Mn,Ni,Pt,Re,Ru,Si,Ta) (Cr,Fe,Mo,Nb,Ta,Ti,V,W) (Al,Co,Cr,Fe,Mn,Mo,Nb, Ni,Pt,Re,Ru,Si,Ta,Ti,V,W)
Spinel	CEF (SLN)	(1)(2)(2)(4)	(Al+3,Co+2,Cr+2,Cr+3,Fe+2,Fe+3,Ni+2)

Name	Model	Lattice Size	Constituent
			(Al+3,Co+3,Cr+3,Fe+2,Fe+3,Va) (Fe+2,Va) (O-2)
Ta2O5_S	CEF (SLN)	(1)	(Ta,Ta2O5)
Ta2O5_S2	CEF (SLN)	(1)	(Ta,Ta2O5)
TaV2_C14	CEF (SLN)	(2)(1)	(Ta,V)(Ta,V)
TaV2_C15	CEF (SLN)	(2)(1)	(Ta,V)(Ta,V)
Tau2_AlNiZr	CEF (SLN)	(1)(2)(1)	(Al)(Ni)(Hf,Zr)
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)
Ti2CS	CEF (ST3)	(2)(1)(1)	(Ti)(C)(S)
Ti2S	CEF (SLN)	(2)(1)	(Ti)(S,Va)
Ti3O2	CEF (ST2)	(3)(2)	(Ti)(O)
Ti3O5	CEF (ST2)	(3)(5)	(Ti)(O)
Ti3P	CEF (ST2)	(3)(1)	(Ti)(P)
Ti4O7	CEF (ST2)	(4)(7)	(Ti)(O)
Ti4P3	CEF (ST2)	(4)(3)	(Ti)(P)
Ti5Al11	CEF (ST2)	(17)(8)	(Al)(Ti)
Ti5O9	CEF (ST2)	(5)(9)	(Ti)(O)
Ti5P3	CEF (SLN)	(0.61)(0.39)	(Ti)(P,Ti)
Ti63P37	CEF (ST2)	(0.63)(0.37)	(Ti)(P)
Ti6O11	CEF (ST2)	(6)(11)	(Ti)(O)
Ti7O13	CEF (ST2)	(7)(13)	(Ti)(O)
Ti8O15	CEF (ST2)	(8)(15)	(Ti)(O)

Name	Model	Lattice Size	Constituent
Ti8S10	CEF (ST2)	(8)(10)	(Ti)(S)
Ti8S3	CEF (ST2)	(8)(3)	(Ti)(S)
Ti8S9	CEF (ST2)	(8)(9)	(Ti)(S)
Ti9O17	CEF (ST2)	(9)(17)	(Ti)(O)
TiAl2	CEF (ST2)	(2)(1)	(Al)(Ti)
TiOx	CEF (SLN)	(1)(1)(1)	(Ti+2,Ti+3,Va)(Ti,Va)(O-2)
TiP	CEF (SLN)	(1)(1)	(Ti)(P,Ti)
TiP2	CEF (ST2)	(1)(2)	(Ti)(P)
TiS2	CEF (SLN)	(1)(2)	(Ti)(S,Va)
TiS3	CEF (SLN)	(1)(3)	(Ti)(S,Va)
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)
V3B4	CEF (ST2)	(3)(4)	(V)(B)
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)

Name	Model	Lattice Size	Constituent
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)
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)
Y2O3_cub	CEF (SLN)	(2)(3)(1)	(Mn+3,Y+3,Va)(O-2)(O-2,Va)
Y2O3_hex	CEF (SLN)	(2)(3)(1)	(Y+3,Zr+4)(O-2)(O-2,Va)
Zr2O	CEF (ST2)	(2)(1)	(Zr)(O)
Zr3O	CEF (ST2)	(3)(1)	(Zr)(O)
Zr6O	CEF (ST2)	(6)(1)	(Zr)(O)
ZrO2_Cubic	CEF (SLN)	(1)(2)	(Hf,Zr)(O,Va)
ZrO2 _Tetra-gonal	CEF (SLN)	(1)(2)	(Hf,Zr)(O,Va)
alpha_Al3Y	CEF (ST2)	(0.75)(0.25)	(Al)(Y)
m_Ni4B3	CEF (ST2)	(0.564) (0.436)	(Ni)(B)
o_Ni4B3	CEF (ST2)	(0.586) (0.414)	(Ni)(B)