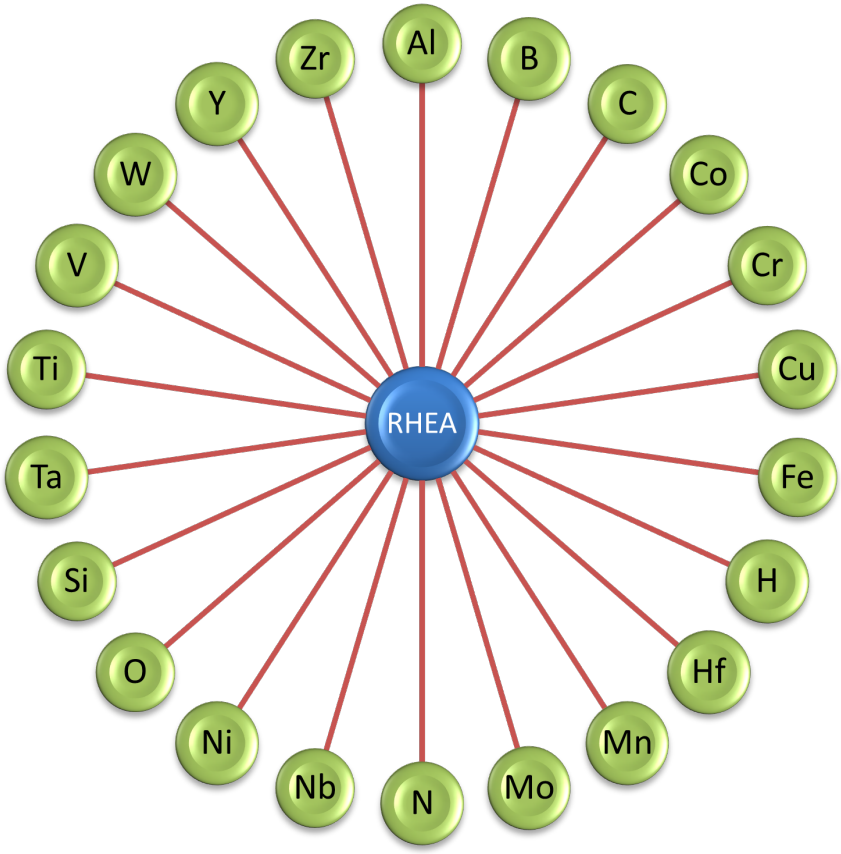
Pandat™ 2024

Database Manual

CompuTherm LLC

PanRHEA

Database for multi-component refractory high entropy alloys (RHEA)



PANDAT™
SOFTWARE

Contents

1 Thermodynamic Database

1.1 Components (22)

Total of **22** components are included in the database as listed here:

Major alloying elements: Al, Co, Cr, Cu, Fe, Hf, Mn, Mo, Nb, Ni, Si, Ta, Ti, V, W, Y, and Zr

Minor alloying element: B, C, H, N and O

1.2 Suggested Composition Range

The suggested composition range for each element is listed in Table 1.1. The suggested composition range is estimated based on the assess subsystems as given in Section 1.4 and the validation in multi-component range as illustrated in Section 1.5 .

Table 1.1: Suggested composition range

Elements	Composition Range (wt.%)
Hf, Mo, Nb, Ta, V, W, Y, Zr	0 ~ 100
Al, Co, Cr, Cu, Fe, Mn, Ni, Si, Ti	0 ~ 50
B, C, H, N, O	0 ~ 10

1.3 Phases

Total of **509** 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 PanRHEA2024: 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
Al6MoZr	(6)(1)(1)	(Al)(Mo)(Zr)
AlNbZr	(1)(1)(1)	(Al)(Nb)(Zr)
B9Cr9Ta2	(9)(9)(2)	(B)(Cr)(Ta)
Bcc	(1)(3)	(Al,B,Co,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Si,Ta,Ti,V,W,Y,Zr)(B,C,H,N,O,Va)
CrNbSi_T1	(6)(5)	(Cr,Nb)(Si)
Fcc	(1)(1)	(Al,B,Co,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Si,Ta,Ti,V,W,Y,Zr)(B,C,H,N,O,Va)
Hcp	(1)(0.5)	(Al,Co,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Si,Ta,Ti,V,W,Zr)(B,C,O,Va)
Hf2Mo3Si	(2)(3)(1)	(Hf)(Mo)(Si)
Hf2Nb2V	(2)(1)	(Hf,Nb)(V)
HfMoSi	(1)(1)(1)	(Hf)(Mo)(Si)
Laves_C14	(2)(1)	(Al,Co,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Si,Ta,Ti,V,Zr)(Al,Co,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Ta,Ti,V,W,Y,Zr)
M5Si3_tI32	(0.625)(0.375)	(Cr,Fe,Hf,Mo,Nb,Si,Ta,Ti,V,W,Zr)(Al,B,Mo,Nb,Si)
Mo3Si5Zr2	(3)(5)(2)	(Mo)(Si)(Zr)
MoSiZr	(1)(1)(1)	(Mo)(Si)(Zr)

Name	Lattice Size	Constituent
Si2TiV	(1)(1)	(Si)(Ti,V)
Sigma	(8)(4)(18)	(Al,Co,Cr,Cu,Fe,Mn,Ni,Si,Ta,Ti) (Cr,Fe,Hf,Mo,Nb,Si,Ta,Ti,V,W,Zr) (Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Si, Ta,Ti,V,W,Zr)(B,Va)
T_AlCoMo	(2.72)(0.28)(1)	(Al)(Co)(Mo)
Ti4Al3Nb	(0.5) (0.375) (0.125)	(Ti)(Al)(Nb)

1.4 Assessed Subsystems

A total of **423** subsystems, including 219 binary and 204 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 (219)

Al-B(10)	Al-C(10)	Al-Co(10)	Al-Cr(10)	Al-Cu(10)	Al-Fe(10)	Al-H(10)
Al-Hf(10)	Al-Mn(10)	Al-Mo(10)	Al-N(10)	Al-Nb(10)	Al-Ni(10)	Al-O(10)
Al-Si(10)	Al-Ta(10)	Al-Ti(10)	Al-V(10)	Al-W(10)	Al-Y(10)	Al-Zr(10)
B-C(10)	B-Co(10)	B-Cr(10)	B-Cu(10)	B-Fe(10)	B-Hf(10)	B-Mn(10)
B-Mo(10)	B-N(10)	B-Nb(10)	B-Ni(10)	B-O(10)	B-Si(10)	B-Ta(10)
B-Ti(10)	B-V(10)	B-W(10)	B-Y(10)	B-Zr(10)	C-Co(10)	C-Cr(10)
C-Fe(10)	C-Hf(10)	C-Mn(10)	C-Mo(10)	C-Nb(10)	C-Ni(10)	C-Si(10)
C-Ta(10)	C-Ti(10)	C-V(10)	C-W(10)	C-Y(10)	C-Zr(10)	Co-Cr(10)
Co-Cu(10)	Co-Fe(10)	Co-H(10)	Co-Hf(10)	Co-Mn(10)	Co-Mo(10)	Co-N(10)
Co-Nb(10)	Co-Ni(10)	Co-O(10)	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-H(10) Cr-Hf(10)
Cr-Mn(10) Cr-Mo(10) Cr-N(10) Cr-Nb(10) Cr-Ni(10) Cr-O(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-H(10) Cu-Hf(10) Cu-Mn(10) Cu-Mo(10) Cu-Nb(10) Cu-Ni(10) Cu-O(10)
Cu-Si(10) Cu-Ta(10) Cu-Ti(10) Cu-V(10) Cu-W(10) Cu-Y(10) Cu-Zr(10)
Fe-H(10) Fe-Hf(10) Fe-Mn(10) Fe-Mo(10) Fe-N(10) Fe-Nb(10) Fe-Ni(10)
Fe-O(10) Fe-Si(10) Fe-Ta(10) Fe-Ti(10) Fe-V(10) Fe-W(10) Fe-Y(10)
Fe-Zr(10) H-Hf(5) H-Mn(10) H-Mo(10) H-Nb(5) H-Ni(10) H-Si(10)
H-Ta(5) H-Ti(10) H-V(8) H-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) Hf-Zr(10) Mn-Mo(10) Mn-N(10) Mn-Nb(10) Mn-Ni(10)
Mn-O(10) Mn-Si(10) Mn-Ta(10) Mn-Ti(10) Mn-V(10) Mn-W(8) Mn-Y(10)
Mn-Zr(10) Mo-N(10) Mo-Nb(10) Mo-Ni(10) Mo-O(10) Mo-Si(10) Mo-Ta(10)
Mo-Ti(10) Mo-V(10) Mo-W(10) Mo-Y(10) Mo-Zr(10) N-Nb(10) N-Ni(8)
N-Si(10) N-Ta(10) N-Ti(10) N-V(10) N-W(10) N-Zr(10) Nb-Ni(10)
Nb-O(10) Nb-Si(10) Nb-Ta(10) Nb-Ti(10) Nb-V(10) Nb-W(10) Nb-Y(10)
Nb-Zr(10) Ni-O(10) Ni-Si(10) Ni-Ta(10) Ni-Ti(10) Ni-V(10) Ni-W(10)
Ni-Y(10) Ni-Zr(10) O-Si(10) O-Ta(10) O-Ti(10) O-V(10) O-W(10)
O-Y(10) O-Zr(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-Y(10)
W-Zr(10) Y-Zr(10)

Ternary Systems (204)

Al-B-Cr(10) Al-B-Mo(10) Al-B-Nb(10) Al-B-Si(10) Al-B-Ti(10) Al-B-V(10)
Al-B-Zr(10) Al-Co-Cr(10) Al-Co-Cu(10) Al-Co-Fe(10) Al-Co-Hf(8) Al-Co-Mn(10)
Al-Co-Mo(10) Al-Co-Nb(10) Al-Co-Ni(10) Al-Co-Si(10) Al-Co-Ti(10) Al-Co-V(10)
Al-Co-W(10) Al-Co-Zr(10) Al-Cr-Mo(10) Al-Cr-Nb(10) Al-Cr-Ni(10) Al-Cr-Si(10)
Al-Cr-Ti(10) Al-Fe-Ni(10) Al-Hf-Nb(5) Al-Hf-Si(10) Al-Hf-Ti(10) Al-Mo-Nb(10)

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

Si-Ta-W(10) Si-Ti-V(10) Si-Ti-Zr(10) Ta-Ti-V(10) Ta-Ti-Zr(10) Ti-V-Zr(10)

1.5 Database Validation and Application

The PanRHEA database is the first commercial database for alloy design and processing optimization of refractory high entropy alloys (RHEA). It has been validated by a large amount of experimental data.

Senkov et al. [2010Sen] investigated two RHEAs W-Nb-Mo-Ta and W-Nb-Mo-Ta-V at the equiatomic ratio. Experimental characterizations of both alloys show single- Bcc microstructure. Figure 1.1 shows the calculated phase stability of these two alloys using the current PanRHEA database.

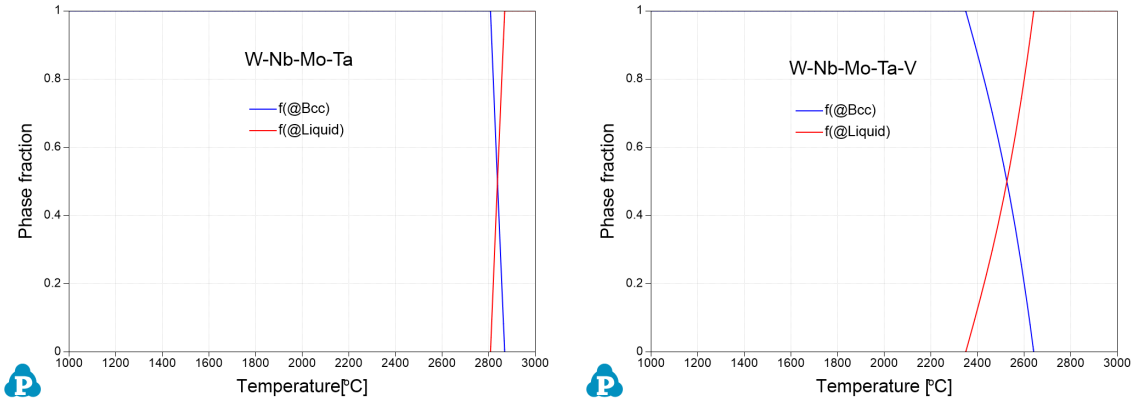


Figure 1.1: Equilibrium calculations of RHEAs: WNbMoTa and WNbMoTaV

Yao et al. [2018Yao] evaluated the phase stablity of a $Hf_{0.5}Nb_{0.5}Ta_{0.5}Ti_{1.5}Zr$ RHEA after annealing for two weeks at 500-900 °C. Microstructural analyses show that the RHEA is a single-phase solid solution after recrystallization at 1000 °C for 3 hours and remains in this state after a subsequent anneal at 900 °C for two weeks. However, it is unstable and forms other intermetallic phases at lower temperatures. After the anneal at 500 °C, the RHEA decomposes into multi-phase microstructures: Ti-rich Hcp phase, Bcc#1 enriches of Hf and Zr, and Bcc#2 enriches of Nb and Ta. Figure 1.2 shows the calculated phase equilibrium of the $Hf_{0.5}Nb_{0.5}Ta_{0.5}Ti_{1.5}Zr$ vs. temperature using the PanRHEA database. Single Bcc phase is stable within a large temperature range and three phases (Bcc#1+Bcc#2+Hcp) coexist at 500 °C, which is consistent with the experimental observations well.

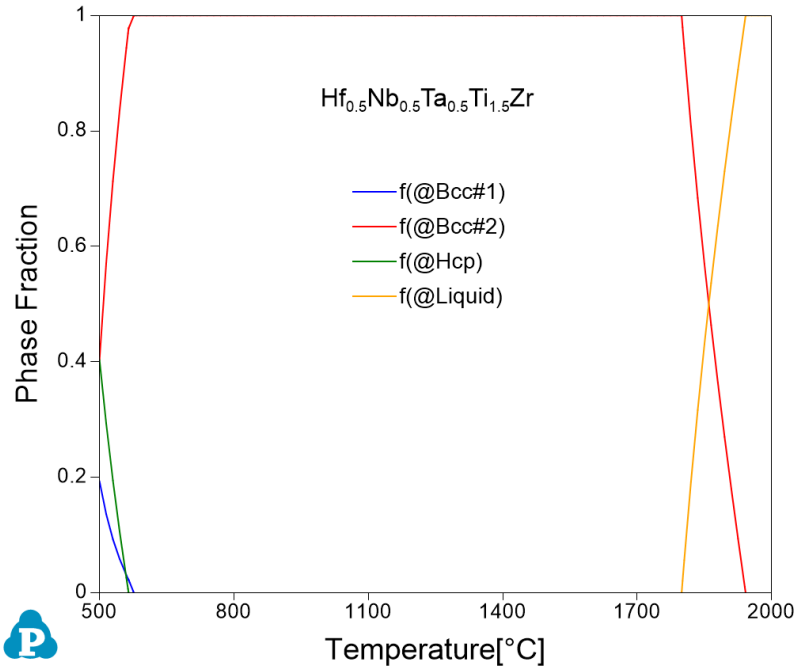


Figure 1.2: Equilibrium calculation of the $Hf_{0.5}Nb_{0.5}Ta_{0.5}Ti_{1.5}Zr$ RHEA alloy

2 Mobility Database

PanRHEA2024_MB is an atomic mobility database for refractory high entropy alloys (RHEA), which is compatible with the `PanRHEA2024_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 color represents the following meaning:

: Validated
: Estimated
: No data

Table 2.1: Assessed self-diffusivity of pure elements with different crystal structures

	Al	Co	Cr	Cu	Fe	Hf	Mn	Mo	Nb	Ni	Si	Ta	Ti	V	W	Zr
Bcc																
Fcc																
Hcp																

2.3 Assessed Systems

In addition to the assessed self-diffusivities shown above, the impurity diffusion data for all included elements in the current `PanRHEA2024_MB` database are also assessed. In the following, the assessed chemical-diffusivity within the binary and ternary systems for the Bcc and Fcc phases are listed, respectively.

Fcc Phase

Al-Co	Al-Cu	Al-Ni	Al-Si	Co-Cr	Co-Cu	Co-Fe	Co-Ni	Cr-Fe	Cr-Ni
Cu-Fe	Cu-Si	Cu-Ti	Fe-Mn	Fe-Ni	Fe-Si	Mn-Ni	Ni-Ti	Ni-V	

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

Bcc phase

Al-Fe	Al-Ti	Cr-Fe	Cr-Ti	Fe-Ti	Hf-Zr	Mo-Nb	Mo-Ta	Mo-Ti	Mo-W
Mo-Zr	Nb-Ta	Nb-Ti	Nb-V	Nb-W	Nb-Zr	Ta-Ti	Ta-W	Ti-V	Ti-Zr
V-Zr									

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

2.4 Database Validation

The simulated concentration profiles of a series of refractory alloys are shown below to validate the current `PanRHEA2024_MB` database.

Figure 2.1 shows the calculated inter-diffusion coefficients of Nb within the Bcc Nb-X (X=W, Zr) binary systems using the current `PanRHEA_MB` database. It indicates that our calculations can well describe the experimental data from literature [2013Liu, 2008Liu].

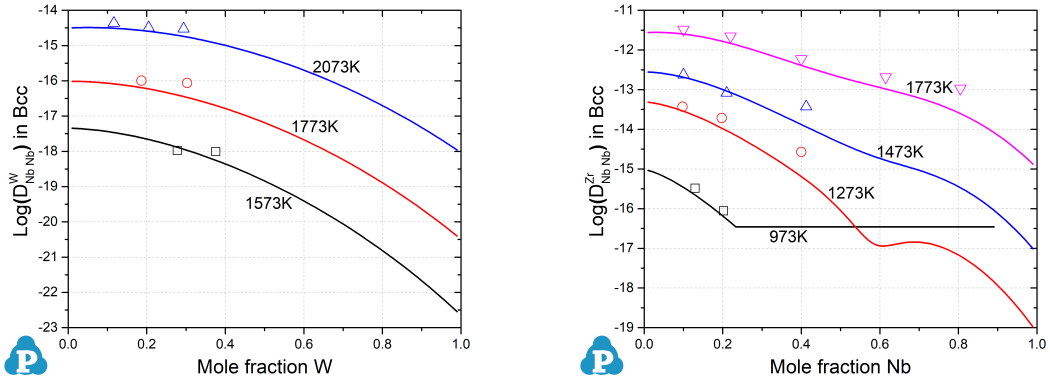


Figure 2.1: Comparison of the calculated inter-diffusion coefficients of Nb in the Bcc Nb-W and Nb-Zr alloys with experimental measurements of [2013Liu] and [2008Liu], respectively

Figure 2.2 shows the simulated concentration profiles of Mo-Ta and Mo-W binary alloys at 2173K and 2318K, respectively. Good agreement between the calculations and experimental data validates the reliability of the current `PanRHEA_MB` database.

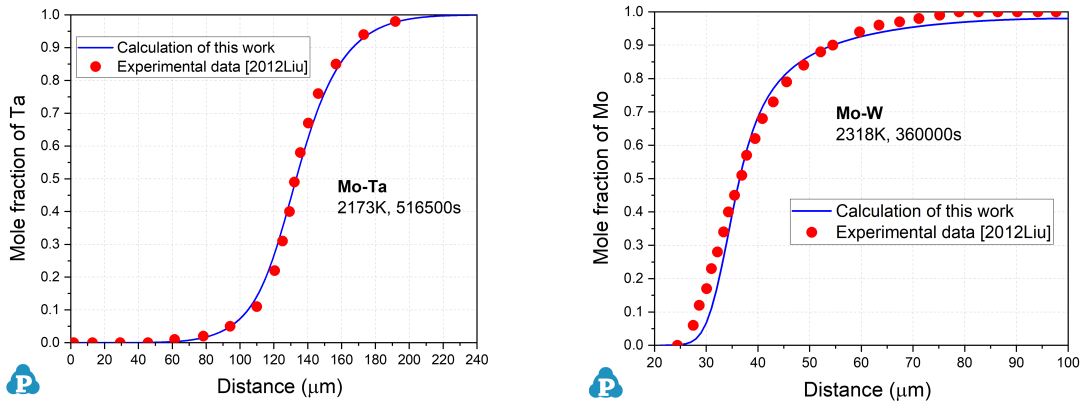


Figure 2.2: Comparison of the simulated concentration profiles of Bcc Mo-Ta and Mo-W binary alloys with experimental measurements of [2012Liu]

3 Thermophysical Property Database

The thermophysical property database **PanRHEA2024_ TP** is compatible with the `PanRHEA2024_ TH` thermodynamic database and suitable for the simulation of thermophysical properties of refractory high entropy alloys(RHEA). 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 **509** phases assessed in the `PanRHEA2024_ TH` database. It is used to calculate the density, thermal expansion, solidification shrinkage of the alloys.

Figure 3.1 shows the calculated molar volume of Bcc Mo-Ti and Nb-Ti binary alloys at room temperature with experimental data from Ref. [2016Yan]. One can see that the calculated results using the current `PanREHA_ MV` database can well describe the experimental measurements.

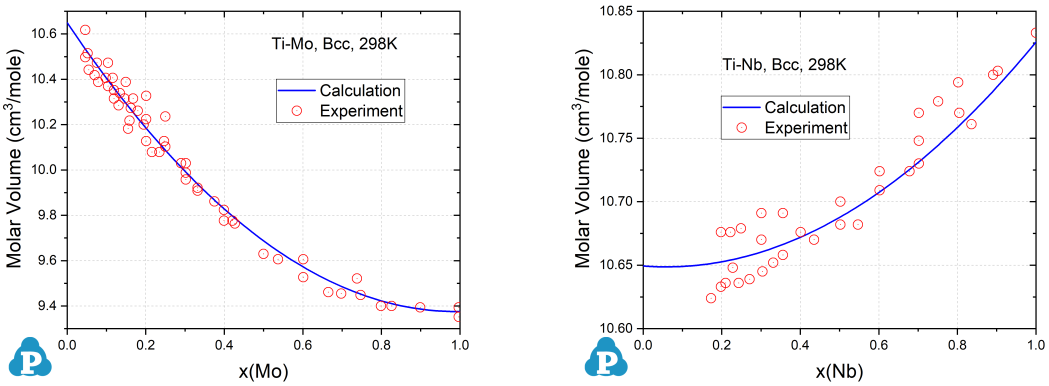


Figure 3.1: Calculated molar volume of Bcc Mo-Ti and Nb-Ti alloys at 298K with experimental data [2016Yan]

3.2 Surface Tension

The surface tension of the liquid phase is added into the property database. Figure 3.2 shows the surface tension of the HfNbTaTiZr refractory high entropy alloy.

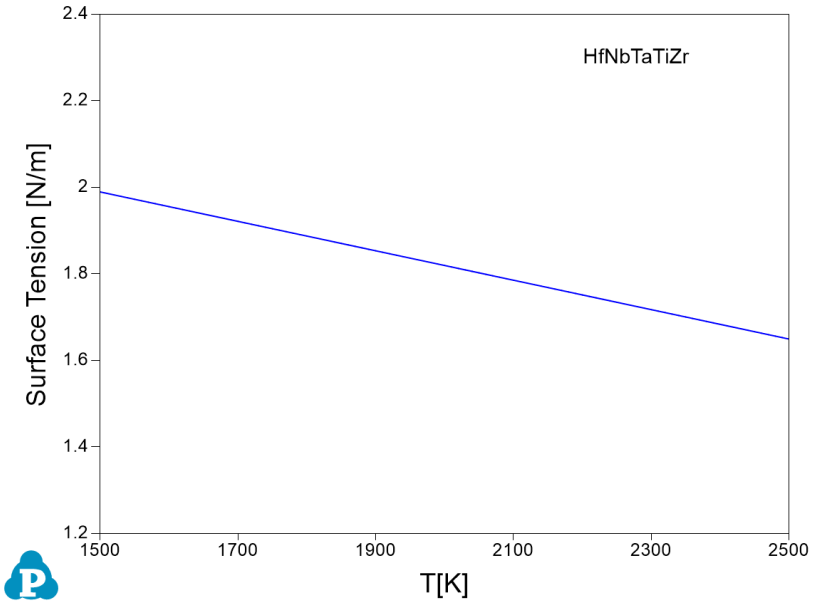


Figure 3.2: Surface tension of HfNbTaTiZr alloy

3.3 Viscosity

The viscosity of the liquid phase is added into the property database. Figure 3.3 shows the viscosity of the HfNbTaTiZr refractory high entropy alloy.

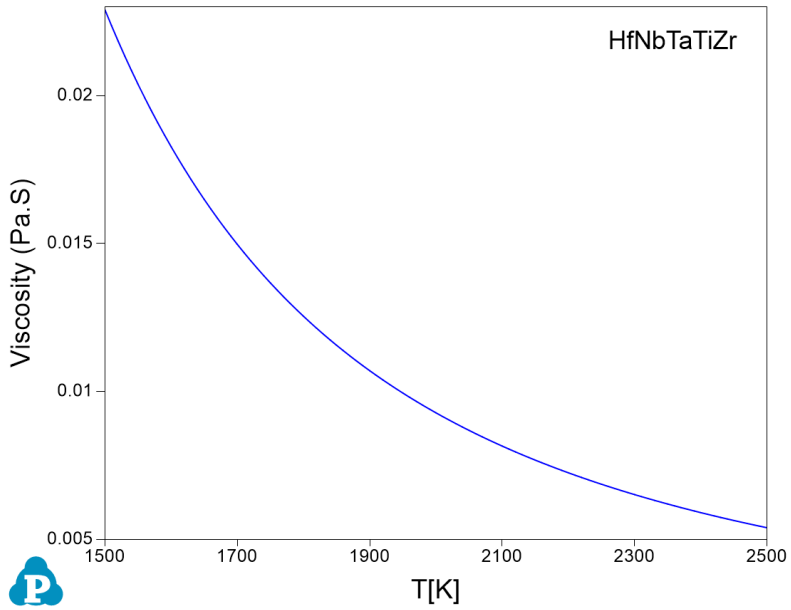


Figure 3.3: Viscosity of the HfNbTaTiZr alloy

4 References

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PanRHEA2024: List of Phases

Phases (**509**)

Name	Model	Lattice Size	Constituent
A15	CEF (SLN)	(0.75)(0.25) (0.05)	(Al,Cr,Fe,Hf,Mo,Nb,Si,Ta,Ti,V,Zr) (Al,Co,Cr,Mo,Nb,Si,Ti,V)(B,Va)
A_Co59Si26V15	CEF (ST3)	(0.59)(0.26) (0.15)	(Co)(Si)(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 (SLN)	(10)(1)	(Al)(Mo,V)
Al11Co6Si6	CEF (ST3)	(11)(6)(6)	(Al)(Co)(Si)
Al11Cr2	CEF (SLN)	(10)(1)(2)	(Al)(Al)(Cr,Mn)
Al11Mn4	CEF (SLN)	(11)(4)	(Al)(Fe,Mn)
Al11Mn4_HT	CEF (SLN)	(29)(10)	(Al,Mn)(Mn)
Al11Ti5	CEF (SLN)	(17)(8)	(Al)(Mo,Ti)
Al12Fe7Mo	CEF (ST3)	(0.45)(0.4) (0.15)	(Al)(Fe)(Mo)
Al12Mn	CEF (SLN)	(12)(1)	(Al)(Fe,Mn)
Al12Mo	CEF (SLN)	(12)(1)	(Al)(Mo,V)
Al12W	CEF (ST2)	(12)(1)	(Al)(W)
Al13Co4	CEF (ST2)	(13)(4)	(Al)(Co)
Al13Cr2	CEF (ST2)	(13)(2)	(Al)(Cr)
Al13M4	CEF (SLN)	(0.6275)	(Al,Cu)(Co,Cr,Fe,Mn,Ni,Si,V)

Name	Model	Lattice Size	Constituent
		(0.235) (0.1375)	(Al,Cu,Si,Va)
Al15_FeMn3Si2	CEF (SLN)	(16)(4)(1)(2)	(Al)(Fe,Mn)(Si)(Al,Si)
Al16Co7Zr6	CEF (ST3)	(16)(7)(6)	(Al)(Co)(Zr)
Al16Mo3Nb	CEF (ST3)	(0.8)(0.15) (0.05)	(Al)(Mo)(Nb)
Al17Mo4	CEF (SLN)	(17)(4)	(Al)(Mo,V)
Al22Mo5	CEF (SLN)	(22)(5)	(Al)(Mo,V)
Al23V4	CEF (SLN)	(23)(4)	(Al,Si)(Mo,V)
Al25Co10Si7	CEF (ST3)	(25)(10)(7)	(Al)(Co)(Si)
Al2CoTi	CEF (SLN)	(3)(1)	(Al,Ti)(Co)
Al2CoZr6	CEF (ST3)	(2)(1)(6)	(Al)(Co)(Zr)
Al2Fe	CEF (SLN)	(2)(1)	(Al,Si)(Co,Cr,Fe,Mn)
Al2Hf	CEF (SLN)	(0.66667) (0.33333)	(Al,Si,Ti)(Hf)
Al2Hf3	CEF (SLN)	(0.4)(0.6)	(Al,Si)(Hf)
Al2NbV	CEF (ST3)	(0.5)(0.25) (0.25)	(Al)(Nb)(V)
Al2Ti	CEF (SLN)	(2)(1)	(Al,Cr)(Mo,Nb,Ti,Zr)
Al2W	CEF (ST2)	(2)(1)	(Al)(W)
Al2Zr3	CEF (SLN)	(2)(3)	(Al)(Nb,Ti,Zr)
Al3B48Si	CEF (ST3)	(3)(48)(1)	(Al)(B)(Si)
Al3Co	CEF (SLN)	(3)(1)	(Al,Si)(Co)
Al3Co3Si4	CEF (ST3)	(3)(3)(4)	(Al)(Co)(Si)
Al3CoCu	CEF (ST3)	(3)(1)(1)	(Al)(Co)(Cu)
Al3Hf2	CEF (SLN)	(0.6)(0.4)	(Al,Si)(Hf)

Name	Model	Lattice Size	Constituent
Al3Hf4	CEF (SLN)	(0.42857) (0.57143)	(Al,Si)(Hf)
Al3Hf_alpha	CEF (SLN)	(0.75)(0.25)	(Al,Si)(Hf)
Al3Mo	CEF (SLN)	(3)(1)	(Al)(Mo,V)
Al3Ni	CEF (SLN)	(0.75)(0.25)	(Al)(Ni,V)
Al3Ni5	CEF (ST2)	(0.375)(0.625)	(Al)(Ni)
Al3NiM2	CEF (SLN)	(3)(2)(1)	(Al,Si)(Al,Co,Cu,Ni,V,Zr) (Co,Cu,Ni,Va)
Al3Ta2V	CEF (ST3)	(3)(2)(1)	(Al)(Ta)(V)
Al3V	CEF (SLN)	(3)(1)	(Al)(Mo,V)
Al3Zr	CEF (SLN)	(3)(1)	(Al,Si)(Ti,V,Zr)
Al3Zr2	CEF (SLN)	(3)(2)	(Al,Nb)(Ti,Zr)
Al3Zr4	CEF (SLN)	(3)(4)	(Al)(Nb,Ti,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,Mo,Si)(C)
Al4CoZr	CEF (ST3)	(4)(1)(1)	(Al)(Co)(Zr)
Al4Cr	CEF (SLN)	(4)(1)	(Al,Si)(Cr)
Al4Mn	CEF (SLN)	(4)(1)	(Al)(Fe,Mn)
Al4Mn_L	CEF (ST2)	(461)(107)	(Al)(Mn)
Al4Mo	CEF (SLN)	(4)(1)	(Al)(Mo,V)
Al4W	CEF (ST2)	(4)(1)	(Al)(W)
Al4Zr5	CEF (ST2)	(4)(5)	(Al)(Zr)
Al5Co2	CEF (SLN)	(5)(2)	(Al,Si)(Co,Fe)

Name	Model	Lattice Size	Constituent
Al5CoCu4	CEF (ST3)	(5)(1)(4)	(Al)(Co)(Cu)
Al5Fe2	CEF (SLN)	(5)(2)	(Al,Si)(Co,Cr,Fe,Mn,Ni,V)
Al5Fe4	CEF (SLN)	(1)	(Al,Fe,Mn)
Al5Mo	CEF (SLN)	(5)(1)	(Al)(Mo,V)
Al5W	CEF (ST2)	(5)(1)	(Al)(W)
Al63Mo37	CEF (SLN)	(63)(37)	(Al)(Mo,Ti)
Al67Cr8Ti25	CEF (SLN)	(0.25)(0.08) (0.67)	(Al,Cr,Ti)(Al,Cr)(Al,Cr,Ti)
Al69Ta39	CEF (SLN)	(0.6389) (0.3611)	(Al,Ta)(Al,Ta)
Al6CoCu3	CEF (ST3)	(6)(1)(3)	(Al)(Co)(Cu)
Al6MoZr	CEF (ST3)	(6)(1)(1)	(Al)(Mo)(Zr)
Al6_FeMn	CEF (SLN)	(6)(1)	(Al)(Fe,Mn)
Al77W23	CEF (ST2)	(77)(23)	(Al)(W)
Al7Co4Si2	CEF (ST3)	(7)(4)(2)	(Al)(Co)(Si)
Al7CoCu2	CEF (ST3)	(7)(1)(2)	(Al)(Co)(Cu)
Al7Nb2Zr4	CEF (ST3)	(6.5)(1.95) (4.55)	(Al)(Nb)(Zr)
Al7V	CEF (SLN)	(7)(1)	(Al)(Mo,V)
Al7W3	CEF (ST2)	(7)(3)	(Al)(W)
Al8Cr5_H	CEF (SLN)	(8)(5)	(Al)(Cr,Ti)
Al8Cr5_L	CEF (SLN)	(8)(5)	(Al,Si)(Cr,Fe,Ti)
Al8FeMnSi2	CEF (ST4)	(16)(2)(2)(3)	(Al)(Fe)(Mn)(Si)
Al8Mn5	CEF (SLN)	(12)(5)(9)	(Al)(Mn)(Al,Mn)
Al8Mo3	CEF (SLN)	(8)(3)	(Al,Ti)(Mo,V)

Name	Model	Lattice Size	Constituent
Al8V5	CEF (SLN)	(8)(5)	(Al)(Mo,Nb,V)
Al9Co2	CEF (SLN)	(9)(2)	(Al,Si)(Co)
Al9Cr4_H	CEF (SLN)	(9)(4)	(Al,Si)(Cr)
Al9Cr4_L	CEF (SLN)	(9)(4)	(Al,Si)(Cr,Fe)
Al9FeNi	CEF (ST3)	(9)(1)(1)	(Al)(Fe)(Ni)
AlB12_Alpha	CEF (ST2)	(1)(12)	(Al)(B)
AlB2Cr2	CEF (ST3)	(0.2)(0.4)(0.4)	(Al)(B)(Cr)
AlB4Cr3	CEF (ST3)	(0.125)(0.5) (0.375)	(Al)(B)(Cr)
AlB7Cr3	CEF (ST3)	(0.09091) (0.6363) (0.2727)	(Al)(B)(Cr)
AlCo2M	CEF (SLN)	(1)(2)(1)	(Al,Nb)(Co)(Al,Co,Nb,Ta)
AlCo2Zr	CEF (ST3)	(1)(2)(1)	(Al)(Co)(Zr)
AlCr2	CEF (SLN)	(1)(2)	(Al,Si)(Cr)
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,V)
AlCu_Theta	CEF (SLN)	(0.667)(0.333)	(Al)(Al,Cu)
AlCu_Zeta	CEF (ST2)	(0.45)(0.55)	(Al)(Cu)
AlHf	CEF (SLN)	(0.5)(0.5)	(Al,Si)(Hf)
AlHfSi	CEF (ST3)	(0.35)(1) (0.65)	(Al)(Hf)(Si)
AlMnSi_Beta	CEF (SLN)	(15)(1)(4)(6)	(Al)(Si)(Al,Si)(Mn)
AlMoSi_C40	CEF (SLN)	(2)(1)	(Al,Si)(Mo)

Name	Model	Lattice Size	Constituent
AlMoSi_C54	CEF (ST3)	(0.434)(0.333) (0.233)	(Al)(Mo)(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)
AlNbZr	CEF (ST3)	(1)(1)(1)	(Al)(Nb)(Zr)
AlSiV	CEF (SLN)	(0.66666) (0.3334)	(Al,Si)(V)
AlZr	CEF (SLN)	(1)(1)	(Al)(Nb,Zr)
AlZr2	CEF (SLN)	(1)(2)	(Al)(Nb,Ti,Zr)
AlZr3	CEF (SLN)	(1)(3)	(Al)(Ti,Zr)
Alpha_AlFeSi	CEF (SLN)	(0.6612)(0.19) (0.0496) (0.0992)	(Al)(Fe,V)(Si)(Al,Si)
Alpha_Co2Si	CEF (SLN)	(2)(1)	(Co,Cr,Fe,Mn,Si,Ti,Zr)(Co,Si)
Alpha_Mn2B	CEF (ST2)	(0.670691) (0.329309)	(Mn)(B)
Alpha_TiMn	CEF (ST2)	(1)(1)	(Mn)(Ti)
Alpha_WB	CEF (SLN)	(1)(1)	(W)(B,Va)
B2	CEF (SLN)	(1)(1)	(Al,Co,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Si, Ta,Ti,W,Zr)(Al,Co,Cr,Cu,Fe,Hf,Mn, Mo,Nb,Ni,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)

Name	Model	Lattice Size	Constituent
B4Mo	CEF (ST2)	(0.8)(0.2)	(B)(Mo)
B5Mo2	CEF (SLN)	(2)(5)	(Mo)(B,Va)
B6O	CEF (ST2)	(6)(1)	(B)(O)
B6Si	CEF (SLN)	(210)(23)(48)	(B)(Si)(B,Si)
B9Cr9Ta2	CEF (ST3)	(9)(9)(2)	(B)(Cr)(Ta)
BCrV	CEF (ST3)	(1)(1.8)(0.2)	(B)(Cr)(V)
BETA_ RHOMBO_B	CEF (SLN)	(93)(12)	(B)(B,Mn,Si,Zr)
BETA_VO	CEF (SLN)	(1)(1)	(V)(O,Va)
B_Co27Si27V46	CEF (ST3)	(0.27)(0.27) (0.46)	(Co)(Si)(V)
B_NSi	CEF (SLN)	(61)(1)(8)	(B)(Si)(B,Si)
Bcc	CEF (SLN)	(1)(3)	(Al,B,Co,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni, Si,Ta,Ti,V,W,Zr)(B,C,O,Va)
Bcc_B2	CEF (SLN)	(0.5)(0.5)(3)	(Al,Co,Cr,Cu,Fe,Hf,Mo,Nb,Si,Ta,Ti, V,Zr)(Al,Co,Cr,Cu,Fe,Hf,Mo,Nb,Si, Ta,Ti,V,Zr)(Va)
Beta_AlFeSi	CEF (SLN)	(0.598)(0.152) (0.1)(0.15)	(Al)(Fe,V)(Si)(Al,Si)
Beta_Co2Si	CEF (SLN)	(2)(1)	(Co,Si)(Co,Si)
Beta_Si4Zr5	CEF (ST2)	(4)(5)	(Si)(Zr)
Beta_TiMn	CEF (ST2)	(0.515)(0.485)	(Mn)(Ti)
Beta_WB	CEF (SLN)	(1)(1)	(W)(B,Va)
CBCC_A12	CEF (SLN)	(1)(1)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Nb,Ni,Si,Ta, Ti,V,Zr)(C,Va)
CUB_A13	CEF (SLN)	(1)(1)	(Al,Co,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Si,

Name	Model	Lattice Size	Constituent
			Ta,Ti,V,Zr)(C,Va)
C_Co34Si27V39	CEF (ST3)	(0.34)(0.27) (0.39)	(Co)(Si)(V)
Cementite	CEF (SLN)	(3)(1)	(Cr,Fe,Mo)(C)
Chi_A12	CEF (SLN)	(24)(10)(24)	(Cr,Fe,Ni)(Cr,Hf,Mo,Nb,Ta,Ti,W,Zr) (Cr,Fe,Mo,Nb,Ni,Ta,W)
Co10Cu57Ti33	CEF (ST3)	(0.57)(0.1) (0.33)	(Cu)(Co)(Ti)
Co16Si7Ti6	CEF (ST3)	(16)(7)(6)	(Co)(Si)(Ti)
Co2Si13Ti5	CEF (ST3)	(2)(13)(5)	(Co)(Si)(Ti)
Co2SiTi	CEF (ST3)	(2)(1)(1)	(Co)(Si)(Ti)
Co3Cr2Si	CEF (ST3)	(3)(2)(1)	(Co)(Cr)(Si)
Co3Cr3Si2	CEF (ST3)	(3)(3)(2)	(Co)(Cr)(Si)
Co3Mn3Mo4	CEF (ST3)	(0.3)(0.3)(0.4)	(Co)(Mn)(Mo)
Co3Si	CEF (ST2)	(0.75)(0.25)	(Co)(Si)
Co3Si2Ti	CEF (ST3)	(3)(2)(1)	(Co)(Si)(Ti)
Co3V	CEF (SLN)	(0.75)(0.25)	(Co,Cr,Fe,V)(Co,Cr,Fe,V)
Co4Cr2Ti	CEF (ST3)	(4)(2)(1)	(Co)(Cr)(Ti)
Co5Cr5Si6	CEF (ST3)	(5)(5)(6)	(Co)(Cr)(Si)
Co7Nb2	CEF (ST2)	(7)(2)	(Co)(Nb)
Co7Ta2	CEF (ST2)	(7)(2)	(Co)(Ta)
CoMo3Si	CEF (ST3)	(1)(3)(1)	(Co)(Mo)(Si)
CoMoZr4	CEF (ST3)	(1)(1)(4)	(Co)(Mo)(Zr)
CoNiTi	CEF (SLN)	(3)(1)	(Co,Ni)(Co,Ni,Ti)
CoSi2Ti	CEF (ST3)	(1)(2)(1)	(Co)(Si)(Ti)

Name	Model	Lattice Size	Constituent
CoSiTi	CEF (ST3)	(1)(1)(1)	(Co)(Si)(Ti)
CoTa2	CEF (SLN)	(1)(2)	(Co,Ta)(Ta)
CoV3	CEF (SLN)	(1)(3)	(Co,Fe)(Cr,V)
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 (SLN)	(0.667)(0.333)	(Cr,V)(B)
Cr3Mn5	CEF (ST2)	(3)(5)	(Cr)(Mn)
Cr3O4	CEF (ST2)	(3)(4)	(Cr)(O)
Cr5Si3B	CEF (ST3)	(5)(3)(1)	(Cr)(Si)(B)
CrB4	CEF (ST2)	(0.2)(0.8)	(Cr)(B)
CrHfSi	CEF (ST3)	(1)(1)(1)	(Cr)(Hf)(Si)
CrNbSi_T1	CEF (SLN)	(6)(5)	(Cr,Nb)(Si)
CrNbSi_T2	CEF (SLN)	(11)(8)	(Cr,Nb)(Si)
CrNbSi_T3	CEF (ST3)	(1)(1)(1)	(Cr)(Nb)(Si)
Cristobalite	CEF (ST2)	(2)(1)	(O)(Si)
Cu2O	CEF (ST2)	(2)(1)	(Cu)(O)
Cu2Ti	CEF (SLN)	(0.666667) (0.333333)	(Co,Cu,Fe,Ni)(Ti)
Cu3Ti2	CEF (SLN)	(0.6)(0.4)	(Cu,Fe,Ni)(Co,Ti)
Cu4Ti	CEF (SLN)	(0.8)(0.2)	(Cu,Ni,Ti)(Cu,Ni,Ti)
Cu4Ti3	CEF (SLN)	(0.57143) (0.42857)	(Co,Cu,Fe,Ni)(Ti)
CuO	CEF (ST2)	(1)(1)	(Cu)(O)
CuTi	CEF (SLN)	(0.5)(0.5)	(Co,Cu,Ni,Ti)(Cu,Ni,Ti,Zr)
CuZr	CEF (SLN)	(1)(1)	(Cu,Ni)(Ti,Zr)

Name	Model	Lattice Size	Constituent
D0_19	CEF (SLN)	(0.75)(0.25) (0.5)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,V,Zr) (Al,Mn,Mo,Nb,Ta,Ti,Zr)(C,Va)
D0_22	CEF (SLN)	(0.75)(0.25) (0.5)	(Al,Cr,Mo,Si,Ti) (Al,Cr,Hf,Mo,Nb,Ta,Ti,V,Zr)(C,Va)
D8_8	CEF (SLN)	(0.5556) (0.3333) (0.1111)	(Hf,Nb,V)(Si,B)(B,Va)
Delta	CEF (SLN)	(3)(1)	(Al,Co,Cr,Fe,Nb,Ni,Ta,Ti) (Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Si,Ta,Ti, W,Zr)
Delta_AlFeSi	CEF (SLN)	(0.4166) (0.1667)(0.25) (0.1667)	(Al)(Fe)(Si)(Al,Si)
Delta_Cu33Si7	CEF (ST2)	(0.825)(0.175)	(Cu)(Si)
Diamond_A4	CEF (SLN)	(1)	(Al,B,C,Si,Ti)
Epsilon_Cu15Si4	CEF (SLN)	(0.789474) (0.210526)	(Cu)(Al,Si)
Eta	CEF (SLN)	(0.75)(0.25)	(Co,Cu,Fe,Ni,Ti) (Al,Cr,Hf,Mo,Nb,Ni,Si,Ta,Ti,V,Zr)
Eta_Cu19Si6	CEF (ST2)	(0.76)(0.24)	(Cu)(Si)
Eta_MC	CEF (SLN)	(1)(1)	(Mo,W)(C,Va)
Fcc	CEF (SLN)	(1)(1)	(Al,B,Co,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni, Si,Ta,Ti,V,W,Zr)(B,C,O,Va)
Fe2Hf_C14	CEF (SLN)	(0.6667) (0.3333)	(Fe)(Fe,Hf)
Fe2Hf_C15	CEF (ST2)	(0.6667) (0.3333)	(Fe)(Hf)

Name	Model	Lattice Size	Constituent
Fe2Hf_C36	CEF (ST2)	(0.6667) (0.3333)	(Fe)(Hf)
Fe2Si	CEF (ST2)	(2)(1)	(Fe)(Si)
FeHf2	CEF (ST2)	(0.3333) (0.6667)	(Fe)(Hf)
FeSi2_H	CEF (ST2)	(3)(7)	(Fe)(Si)
FeSi2_L	CEF (ST2)	(1)(2)	(Fe)(Si)
FeZr3	CEF (SLN)	(1)(3)	(Al,Fe,Zr)(Fe,Zr)
Gamma_AlFeSi	CEF (SLN)	(0.5)(0.2)(0.1) (0.2)	(Al)(Fe)(Si)(Al,Si)
Gamma_ Cu56Si11	CEF (ST2)	(0.835821) (0.164179)	(Cu)(Si)
Gamma_H	CEF (SLN)	(4)(1)(8)	(Al,Si)(Al,Cu)(Cu)
Gamma_double_ prime	CEF (SLN)	(3)(1)	(Al,Co,Cr,Fe,Nb,Ni,Ta,Ti) (Al,Co,Cr,Fe,Hf,Mo,Nb,Ni,Ta,Ti,W)
Gas	GAS	(1)	(Al,AlO,Al2O,AlO2,Al2O2,B,B1O1, B1O2,B2,B2O1,B2O2,B2O3,C1O1, C1O2,Fe,FeO,FeO2,Fe2,Hf,HfO, HfO2,Mn,MnO,Mn1O2,Mo,MO1O1, MO1O2,MO1O3,MO2,MO2O6, MO3O9,MO4O12,MO5O15,O,SiO, O2,SiO2,Si2O2,O3,Si,Si2,Si3,TaO, O,O2,TaO2,Ta,Ti,TiO,TiO2,ZrO, ZrO2,Zr,Zr2)
Graphite	CEF (SLN)	(1)	(B,C)
H_CoMnSi	CEF (ST3)	(0.5)(0.25) (0.25)	(Co)(Mn)(Si)

Name	Model	Lattice Size	Constituent
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,Mn,Mo,Nb,Ni,Si, Ta,Ti,V,W,Zr)(B,C,O,Va)
Hf2Mo3Si	CEF (ST3)	(2)(3)(1)	(Hf)(Mo)(Si)
Hf2Nb2V	CEF (SLN)	(2)(1)	(Hf,Nb)(V)
Hf3Nb2V5	CEF (ST3)	(3)(2)(5)	(Hf)(Nb)(V)
Hf9Mo4B	CEF (ST3)	(9)(4)(1)	(Hf)(Mo)(B)
HfMn	CEF (ST2)	(0.5)(0.5)	(Hf)(Mn)
HfMn2	CEF (SLN)	(1)(2)	(Hf,Mn)(Hf,Mn)
HfMoSi	CEF (ST3)	(1)(1)(1)	(Hf)(Mo)(Si)
HfNiTi_Tao	CEF (SLN)	(11)(14)	(Ni)(Hf,Ti)
HfO2_S	CEF (SLN)	(1)	(Hf,HfO2,Ta)
HfO2_S2	CEF (SLN)	(1)	(Hf,HfO2)
HfO2_S3	CEF (SLN)	(1)	(Hf,HfO2)
HfTaO	CEF (SLN)	(6)(1)	(HfO2,Ta2O5)(HfO2,Ta2O5)
J_Co45Si40V15	CEF (ST3)	(0.45)(0.4) (0.15)	(Co)(Si)(V)
Ksi_Carbide	CEF (SLN)	(3)(1)	(Cr,Fe,Mo,W)(C)
L10_TiAl	CEF (SLN)	(1)(1)(2)	(Al,Cr,Mn,Mo,Nb,Ta,Ti,V,W,Zr) (Al,Cr,Mn,Mo,Nb,Ta,Ti,V,W,Zr) (C,O,Va)
L12_FCC	CEF (SLN)	(0.75)(0.25) (1)	(Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Si, Ta,Ti,V,W,Zr)(Al,Co,Cr,Fe,Hf,Mn,Mo, Nb,Ni,Si,Ta,Ti,V,W,Zr)(Va)
L_CoMnSi	CEF (ST3)	(0.4433)	(Co)(Mn)(Si)

Name	Model	Lattice Size	Constituent
		(0.3333) (0.2233)	
L_Sigma	CEF (SLN)	(8)(4)(18)	(Mn,Ni)(Cr)(Cr,Mn)
Laves_C14	CEF (SLN)	(2)(1)	(Al,Co,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Si,Ta,Ti,V,Zr)(Al,Co,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Ta,Ti,V,W,Zr)
Laves_C15	CEF (SLN)	(2)(1)	(Al,Co,Cr,Cu,Fe,Hf,Mo,Nb,Ni,Ta,Si,Ti,V,W,Zr)(Al,Co,Cr,Cu,Fe,Hf,Mo,Nb,Ni,Ta,Ti,V,W,Zr)
Laves_C36	CEF (SLN)	(2)(1)	(Al,Co,Cr,Cu,Hf,Fe,Mn,Mo,Nb,Ni,Si,Ta,Ti,V,Zr)(Al,Co,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Si,Ta,Ti,V,Zr)
Liquid	CEF (SLN)	(1)	(Al,B,C,Co,Cr,Cu,Fe,Hf,Mn,Mo,Nb,Ni,Si,Ta,Ti,V,W,Zr,O,Al2O3,CoO,Co2O3,Cr2O3,CuO,Cu2O,Cu2O3,FeO,FeO3/2,HfO2,MnO,Mn2/3O,NbO,NbO2,Nb2O5,NiO,SiO2,Ta2O5,TiO,TiO3/2,TiO2,VO,VO2,VO3/2,VO5/2,WO2,WO3,Zr1/2O)
Liquid_Oxide	CEF (SLN)	(1)	(Al2O3,B6O,B2O3,Cr2O3,MO1O2,MO1O3,SiO2,VO5/2)
M10X7_oS68	CEF (SLN)	(10)(7)	(Al,Cu,Fe,Ni)(Hf,Ti,Zr)
M11X2_mS36	CEF (SLN)	(11)(2)	(Co,Fe)(Hf,Zr)
M11X9_tI40	CEF (SLN)	(11)(9)	(Cu,Ni)(Hf,Ti,Zr)
M21X8_aP29	CEF (SLN)	(21)(8)	(Cu,Ni)(Hf,Zr)
M23C6	CEF (SLN)	(20)(3)(6)	(Co,Cr,Fe,Mn,Ni,V) (Co,Cr,Fe,Mn,Mo,Nb,Ni,Ta,Ti,V,W) (B,C)

Name	Model	Lattice Size	Constituent
M23X6_cF116	CEF (SLN)	(23)(6)	(Co,Cu,Fe,Si)(Hf,Zr)
M2B3	CEF (SLN)	(2)(3)	(Nb,V)(B)
M2X_tI12	CEF (SLN)	(0.333)(0.667)	(Al,B,Fe,Ni,Si) (Co,Cu,Cr,Fe,Hf,Mn,Mo,Nb, Ni,Ta,Ti,V,W,Zr)
M3B4_oI14	CEF (SLN)	(4)(3)	(B)(Al,Cr,Hf,Mn,Mo,Nb,Ta,Ti,V)
M3C2	CEF (SLN)	(3)(2)	(Cr,Mo,V,W)(C)
M3Si	CEF (SLN)	(0.75)(0.25)	(Hf,Nb,Ti,V,Zr)(Al,Si)
M3X2_tP10	CEF (SLN)	(2)(3)	(Al,B,Si) (Cr,Fe,Hf,Mn,Mo,Nb,Ta,Ti,V,Zr)
M3X_oP16	CEF (SLN)	(3)(1)	(Co,Cr,Fe,Ni)(B,C)
M51X14_hP68	CEF (SLN)	(51)(14)	(Cu,Ni)(Hf,Ti,Zr)
M5B6	CEF (SLN)	(5)(6)	(Al,Nb,Ti,V)(B)
M5C2	CEF (SLN)	(5)(2)	(Fe,Mn,V)(C)
M5Si3_hP16	CEF (SLN)	(3)(5)	(Al,Si)(Cr,Fe,Hf,Mn,Mo,Nb,Ti,V,Zr)
M5Si3_tI32	CEF (SLN)	(0.625)(0.375)	(Cr,Fe,Hf,Mo,Nb,Si,Ta,Ti,V,W,Zr) (Al,B,Mo,Nb,Si)
M5Si4_tP36	CEF (SLN)	(0.555556) (0.444444)	(Cr,Hf,Mo,Nb,Ti,Zr)(Al,Si)
M5X_cF24	CEF (SLN)	(5)(1)	(Cr,Cu,Fe,Ni)(Hf,Ti,Zr)
M6C	CEF (SLN)	(2)(2)(2)(1)	(Co,Fe,Ni)(Cr,Mo,Nb,W) (Co,Cr,Fe,Mo,Nb,Ni,Si,V,W)(C)
M7C3	CEF (SLN)	(7)(3)	(Co,Cr,Fe,Mn,Mo,Nb,Ni,V,W)(B,C)
M7X2_mS36	CEF (SLN)	(7)(2)	(Al,Cr,Cu,Fe,Ni,V)(Cr,Hf,Ti,Zr)
M8X	CEF (SLN)	(8)(1)	(Fe,Ni)(Nb,Ta)
M8X3_oP44	CEF (SLN)	(8)(3)	(Cu)(Hf,Zr)

Name	Model	Lattice Size	Constituent
MB2_hP3	CEF (SLN)	(1)(2)	(Al,Cr,Hf,Mn,Mo,Nb,Ta,Ti,V,Zr,Va) (B,Va)
MNbO4	CEF (SLN)	(1)(1)(4)	(Al,Cr)(Nb)(O)
MSi	CEF (SLN)	(0.5)(0.5)	(Co,Cr,Fe,Mn,Ni,Si,V,Zr) (Al,Co,Cr,Si)
MSi2_hP9	CEF (SLN)	(1)(2)	(Co,Cr,Hf,Mo,Nb,Ni,Si,Ta,Ti,V,Zr) (Al,Cr,Si)
MX2_cF96	CEF (SLN)	(1)(2)	(Co,Cr,Cu,Fe,Hf,Ni,Si,Ti) (Al,Cu,Fe,Hf,Ni,Ti,V,Zr)
MX2_tI6	CEF (SLN)	(1)(2)	(Co,Cu,Fe,Ni)(Al,Hf,Ti,Zr)
MX_oP8	CEF (SLN)	(1)(1)	(Al,B,Si)(Co,Cr,Fe,Hf,Mn,Mo,Nb, Ni,Ta,Ti,V,Zr)
MX_oS8	CEF (SLN)	(1)(1)	(B,Cu,Ni,Si) (Al,Cr,Hf,Mo,Nb,Ni,Ta,Ti,V,Zr)
Mn11Si19	CEF (ST2)	(11)(19)	(Mn)(Si)
Mn3C	CEF (ST2)	(3)(1)	(Mn)(C)
Mn3O4_A	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3O4_B	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3Si	CEF (ST2)	(3)(1)	(Mn)(Si)
Mn3Ti	CEF (ST2)	(3)(1)	(Mn)(Ti)
Mn4Ti	CEF (ST2)	(0.815)(0.185)	(Mn)(Ti)
Mn6Si	CEF (ST2)	(17)(3)	(Mn)(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)
MnNi_Beta	CEF (SLN)	(1)(1)	(Co,Cr,Fe,Mn,Ni)(Co,Cr,Fe,Mn,Ni)

Name	Model	Lattice Size	Constituent
MnTa	CEF (ST2)	(1)(1)	(Mn)(Ta)
Mo2BC	CEF (ST3)	(2)(1)(1)	(Mo)(B)(C)
Mo2Fe21C6	CEF (ST3)	(2)(21)(6)	(Mo)(Fe)(C)
Mo2Mn4C	CEF (ST3)	(2)(4)(1)	(Mo)(Mn)(C)
Mo2Ti	CEF (ST2)	(2)(1)	(Mo)(Ti)
Mo3Al2C	CEF (ST3)	(3)(2)(1)	(Mo)(Al)(C)
Mo3M3C	CEF (SLN)	(3)(3)(1)	(Mo)(Fe,Mn)(C)
Mo3Si5Zr2	CEF (ST3)	(3)(5)(2)	(Mo)(Si)(Zr)
Mo3Ti2	CEF (ST2)	(3)(2)	(Mo)(Ti)
Mo4O11	CEF (ST2)	(1)(2.75)	(Mo)(O)
Mo4Si9Ti7	CEF (SLN)	(0.55)(0.45)	(Mo,Ti)(Si)
Mo4Ti	CEF (ST2)	(4)(1)	(Mo)(Ti)
Mo5Si3C	CEF (ST3)	(4.8)(3)(0.6)	(Mo)(Si)(C)
Mo5Si9Zr6	CEF (ST3)	(5)(9)(6)	(Mo)(Si)(Zr)
Mo5Ti	CEF (ST2)	(5)(1)	(Mo)(Ti)
Mo7Ti	CEF (ST2)	(7)(1)	(Mo)(Ti)
Mo8O23	CEF (ST2)	(1)(2.875)	(Mo)(O)
Mo9AlB10	CEF (ST3)	(0.9)(0.1)(1)	(Mo)(Al)(B)
Mo9O26	CEF (ST2)	(1)(2.889)	(Mo)(O)
Mo9Ti	CEF (ST2)	(9)(1)	(Mo)(Ti)
MoAlB	CEF (ST3)	(1)(1)(1)	(Mo)(Al)(B)
MoO2	CEF (SLN)	(1)(2)	(Mo,O)(Mo,O)
MoO3	CEF (ST2)	(1)	(MO1O3)
MoSi2	CEF (SLN)	(1)(2)	(Mo,Nb,V,W)(Al,Si)
MoSi6Ti2	CEF (SLN)	(1)(2)	(Mo,Ti)(Si)

Name	Model	Lattice Size	Constituent
MoSiZr	CEF (ST3)	(1)(1)(1)	(Mo)(Si)(Zr)
MoTi	CEF (ST2)	(1)(2)	(Mo)(Ti)
MoTi2	CEF (ST2)	(1)(2)	(Mo)(Ti)
MoV2O8	CEF (ST3)	(1)(2)	(MO1O3)(VO5/2)
Mu_Phase	CEF (SLN)	(7)(2)(4)	(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Ta,W) (Co,Cr,Mo,Nb,Ni,Ta,Ti,W) (Co,Cr,Fe,Mo,Nb,Ni,Ta,Ti,W)
Nb2O5	CEF (ST2)	(2)(5)	(Nb)(O)
Nb5Si3	CEF (SLN)	(0.625)(0.375)	(Cr,Hf,Mo,Nb,Si,Ti,V,Zr)(Al,B,Si)
Nb9Si2Cr3	CEF (SLN)	(0.643)(0.143) (0.214)	(Nb)(Si)(Cr,Si)
NbO	CEF (ST2)	(1)(1)	(Nb)(O)
NbO2	CEF (ST2)	(1)(2)	(Nb)(O)
Ni2Cr	CEF (SLN)	(2)(1)	(Ni)(Cr,Mo)
Ni2Si_H	CEF (SLN)	(1)(1)(1)	(Ni)(Ni,Va)(Al,Si)
Ni2Si_L	CEF (SLN)	(2)(1)	(Fe,Ni)(Al,Si)
Ni2Ta	CEF (ST2)	(2)(1)	(Ni)(Ta)
Ni2V	CEF (SLN)	(0.6667) (0.3333)	(Ni)(Al,V)
Ni3Hf_Alpha	CEF (SLN)	(3)(1)	(Ni)(Hf,Ti)
Ni3Hf_Beta	CEF (ST2)	(3)(1)	(Ni)(Hf)
Ni3Si2	CEF (SLN)	(3)(2)	(Fe,Mn,Ni)(Si)
Ni3Si_H	CEF (SLN)	(3)(1)	(Ni)(Al,Si)
Ni3Si_L	CEF (SLN)	(3)(1)	(Ni)(Si,Ti)
Ni3V	CEF (SLN)	(3)(1)	(Fe,Ni,V)(Al,Ni,Ti,V)
Ni4Mo	CEF (ST2)	(4)(1)	(Ni)(Mo)

Name	Model	Lattice Size	Constituent
Ni4W	CEF (ST2)	(4)(1)	(Ni)(W)
Ni5Si2	CEF (SLN)	(5)(2)	(Fe,Ni)(Al,Si)
Ni7Hf3	CEF (ST2)	(7)(3)	(Ni)(Hf)
NiMo	CEF (SLN)	(24)(20)(12)	(Co,Cr,Fe,Ni) (Al,Cr,Fe,Mo,Ni,W)(Mo)
NiTiZr	CEF (SLN)	(1)(1)(1)	(Ni,Ti,Zr)(Ni,Ti,Zr)(Ni,Ti,Zr)
NiV3	CEF (ST2)	(0.25)(0.75)	(Ni)(V)
NiW	CEF (ST2)	(1)(1)	(Ni)(W)
NiW2	CEF (ST2)	(1)(2)	(Ni)(W)
P_Phase	CEF (SLN)	(24)(12)(20)	(Co,Cr,Fe,Ni)(Mo,W) (Co,Cr,Fe,Mo,Ni,W)
Phi	CEF (SLN)	(0.8837) (1.1163)	(Al,Ta,Ti)(Al,Nb,Ta,Ti)
Quartz	CEF (ST2)	(2)(1)	(O)(Si)
R_Co40Si15V45	CEF (ST3)	(0.4)(0.15) (0.45)	(Co)(Si)(V)
R_CoMnSi	CEF (ST3)	(0.2)(0.53) (0.27)	(Co)(Mn)(Si)
R_Phase	CEF (SLN)	(27)(14)(12)	(Co,Cr,Fe,Mn,Mo,Ni,V)(Cr,Mo,W) (Co,Cr,Fe,Mn,Mo,Ni,Si,V,W)
Rutile	CEF (SLN)	(1)(2)	(Mn+4,Ti+3,Ti+4,V+4)(O-2,Va)
Shp_MC	CEF (SLN)	(1)(1)	(Mo,W)(C)
Si2Ti	CEF (SLN)	(2)(1)	(Al,Si)(Cr,Mo,Nb,Ti,V)
Si2TiV	CEF (SLN)	(1)(1)	(Si)(Ti,V)
Si2Zr	CEF (SLN)	(2)(1)	(Si)(Nb,Zr)
Si2Zr3	CEF (SLN)	(2)(3)	(Si)(Nb,Zr)

Name	Model	Lattice Size	Constituent
Si3Ta5_HT	CEF (ST2)	(0.375)(0.625)	(Si)(Ta)
Si3Zr5	CEF (SLN)	(3)(5)	(Al,B,Mo,Si)(Zr)
Si5V6	CEF (SLN)	(0.454545) (0.545455)	(Si)(Cr,V)
SiC	CEF (ST2)	(1)(1)	(C)(Si)
SiTa2	CEF (SLN)	(0.3333) (0.6667)	(Al,Si)(Ta,V)
SiTa3	CEF (SLN)	(0.25)(0.75)	(Si)(Ta,V)
SiZr2	CEF (SLN)	(1)(2)	(Al,Si)(Nb,Ti,Zr)
Sigma	CEF (SLN)	(8)(4)(18) (3.75)	(Al,Co,Cr,Cu,Fe,Mn,Ni,Si,Ta,Ti) (Cr,Fe,Hf,Mo,Nb,Si,Ta,Ti,V,W,Zr) (Al,Co,Cr,Fe,Hf,Mn,Mo,Nb,Ni,Si, Ta,Ti,V,W,Zr)(B,Va)
Spinel	CEF (SLN)	(1)(2)(2)(4)	(Al+3,Co+2,Cr+2,Cr+3, Fe+2,Fe+3,Ni+2) (Al+3,Co+3,Cr+3,Fe+2,Fe+3,Va) (Fe+2,Va)(O-2)
T10_AlFeSi	CEF (ST3)	(0.6)(0.25) (0.15)	(Al)(Fe)(Si)
T11_AlFeSi	CEF (ST3)	(0.6538) (0.2308) (0.1154)	(Al)(Fe)(Si)
T1_AlFeMo	CEF (ST3)	(2.72)(0.28) (1)	(Al)(Fe)(Mo)
T1_AlFeSi	CEF (SLN)	(5)(3)	(Al,Si)(Fe)
T1_Co5Si3V4	CEF (ST3)	(0.4167)(0.25) (0.3333)	(Co)(Si)(V)

Name	Model	Lattice Size	Constituent
T1_CoMnSi	CEF (ST3)	(0.08)(0.64) (0.28)	(Co)(Mn)(Si)
T2_CoMnSi	CEF (ST3)	(0.2456) (0.5088) (0.2456)	(Co)(Mn)(Si)
T3_AlFeSi	CEF (ST3)	(0.55)(0.25) (0.2)	(Al)(Fe)(Si)
T7_AlFeSi	CEF (SLN)	(0.75)(0.25)	(Al,Si)(Fe)
T8_AlFeSi	CEF (SLN)	(0.66667) (0.33333)	(Al,Si)(Fe)
T_AlCoMo	CEF (ST3)	(2.72)(0.28) (1)	(Al)(Co)(Mo)
Ta2B	CEF (ST2)	(2)(1)	(Ta)(B)
Ta2O5_S	CEF (SLN)	(1)	(Ta,Ta2O5)
Ta2O5_S2	CEF (SLN)	(1)	(Hf,Ta,Ta2O5)
Tau1_AlCrSi	CEF (ST3)	(13)(4)(4)	(Al)(Cr)(Si)
Tau1_AlSiZr	CEF (ST3)	(0.35)(0.39) (0.26)	(Al)(Si)(Zr)
Tau1_CoSiZr	CEF (ST3)	(1)(1)(1)	(Co)(Si)(Zr)
Tau2_AlCrSi	CEF (ST3)	(9)(3)(1)	(Al)(Cr)(Si)
Tau2_AlSiZr	CEF (ST3)	(0.65)(0.1) (0.25)	(Al)(Si)(Zr)
Tau2_Co5Si3Zr	CEF (ST3)	(5)(3)(1)	(Co)(Si)(Zr)
Tau3_AlCrSi	CEF (SLN)	(11)(4)	(Al,Si)(Cr)
Tau3_CoSi2Zr	CEF (ST3)	(1)(2)(1)	(Co)(Si)(Zr)
Tau4_AlCrSi	CEF (ST3)	(0.58)(0.315) (0.105)	(Al)(Cr)(Si)

Name	Model	Lattice Size	Constituent
Tau4_CoSi2Zr2	CEF (ST3)	(1)(2)(2)	(Co)(Si)(Zr)
Tau5_Co2Si2Zr	CEF (ST3)	(2)(2)(1)	(Co)(Si)(Zr)
Tau6_Co7Si9Zr4	CEF (ST3)	(7)(9)(4)	(Co)(Si)(Zr)
Tau7_CoSi10Zr9	CEF (ST3)	(1)(10)(9)	(Co)(Si)(Zr)
Ti10O19	CEF (ST2)	(10)(19)	(Ti)(O)
Ti20O39	CEF (ST2)	(20)(39)	(Ti)(O)
Ti3Al2Si5	CEF (ST3)	(1)(0.6)(1.4)	(Ti)(Al)(Si)
Ti3O2	CEF (ST2)	(3)(2)	(Ti)(O)
Ti3O5	CEF (ST2)	(3)(5)	(Ti)(O)
Ti4Al3Nb	CEF (ST3)	(0.5)(0.375) (0.125)	(Ti)(Al)(Nb)
Ti4O7	CEF (ST2)	(4)(7)	(Ti)(O)
Ti5O9	CEF (ST2)	(5)(9)	(Ti)(O)
Ti6O11	CEF (ST2)	(6)(11)	(Ti)(O)
Ti6Si2B	CEF (ST3)	(6)(2)(1)	(Ti)(Si)(B)
Ti7Al5Si14	CEF (ST3)	(7)(5)(14)	(Ti)(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)
Tridymite	CEF (ST2)	(2)(1)	(O)(Si)
V2O	CEF (SLN)	(1)(0.5)	(V)(O,Va)
V2O5	CEF (SLN)	(1)	(VO5/2,MO1O3)
V2O_SS	CEF (SLN)	(1)(0.5)	(V)(O,Va)
V3O	CEF (SLN)	(1)(1)	(V)(O,Va)

Name	Model	Lattice Size	Constituent
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)
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)
VO	CEF (SLN)	(1)(1)	(V)(O,Va)
VO2	CEF (SLN)	(1)(2)	(Hf,Mo,V,W,Zr)(O)
W2B	CEF (ST2)	(2)(1)	(W)(B)
W2B5	CEF (SLN)	(2)(5)	(W)(B,Va)
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)
W_CoMnSi	CEF (ST3)	(0.3333) (0.3333) (0.3333)	(Co)(Mn)(Si)
X_Co52Si20V28	CEF (ST3)	(0.52)(0.2) (0.28)	(Co)(Si)(V)
X_CoMnSi	CEF (ST3)	(0.4)(0.4459)	(Co)(Mn)(Si)

Name	Model	Lattice Size	Constituent
		(0.1541)	
Zr2O	CEF (ST2)	(2)(1)	(Zr)(O)
Zr3O	CEF (ST2)	(3)(1)	(Zr)(O)
Zr6O	CEF (ST2)	(6)(1)	(Zr)(O)
ZrB12	CEF (ST2)	(1)(12)	(Zr)(B)
ZrO2_Cubic	CEF (SLN)	(1)(2)	(Hf,Zr)(O,Va)
ZrO2_Tetragonal	CEF (SLN)	(1)(2)	(Hf,Zr)(O,Va)
alpha_BMo	CEF (SLN)	(0.5)(0.5)	(Mo,Ti,V)(B,Va)
m_Ni4B3	CEF (ST2)	(0.564)(0.436)	(Ni)(B)
o_Ni4B3	CEF (ST2)	(0.586)(0.414)	(Ni)(B)