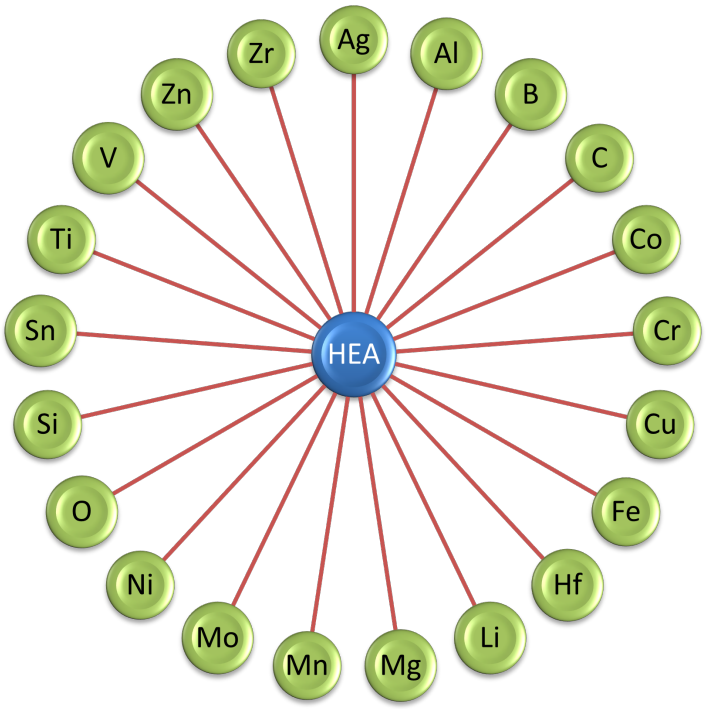
Pandat™ 2024

Database Manual

CompuTherm LLC

PanHEA

Database for multi-component high entropy alloys (HEA)



PANDAT™
SOFTWARE

Contents

1 Thermodynamic Database

1.1 Components (21)

Total of **21** components are included in the database as listed here:

Major alloying elements: Ag, Al, Co, Cr, Cu, Fe, Hf, Li, Mg, Mn, Mo, Ni, O, Si, Sn, Ti, V, Zn and Zr

Minor alloying element: B, C

1.2 Suggested Composition Range

The suggested composition range for each element is listed in Table 1.1.

Table 1.1: Suggested composition range

Elements	Composition Range (wt.%)
Ag, Al, Co, Cr, Cu, Fe, HF, Li, Mg, Mn, Mo, Ni, Si, Sn, Ti, V, Zn, Zr	0 ~ 100
B, C, O	0 ~ 10

1.3 What is new in PanHEA2024

- Addition of the component O
- Improvement of the Al-Ni and Mn-Ti binary descriptions

1.4 Phases

Total of **687** 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 PanAl2024: 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
Al10Cu10Fe	(10)(10)(1)	(Al)(Cu)(Fe)
Al10Fe3Ni	(10)(3)(1)	(Al)(Fe)(Ni)
Al11Co6Si6	(11)(6)(6)	(Al)(Co)(Si)
Al14Mn4Si5	(14)(4)(5)	(Al)(Mn)(Al,Si)
Al16Co7Zr6	(16)(7)(6)	(Al)(Co)(Zr)
Al17Cr2Mg4	(21)(2)	(Al,Mg)(Cr)
Al20Cu2Mn3	(0.8)(0.08)(0.12)	(Al)(Cu)(Mn)
Al23CuFe4	(23)(1)(4)	(Al)(Cu)(Fe)
Al2Mn2Si3	(2)(2)(3)	(Al)(Mn)(Si)
Al3Co3Si4	(3)(3)(4)	(Al)(Co)(Si)
Al3CoCu	(3)(1)(1)	(Al)(Co)(Cu)
Al3Mn4Si2	(3)(4)(2)	(Al)(Mn)(Si)
Al6Cu2Fe	(6)(2)(1)	(Al)(Cu)(Fe)
Al6Cu3Ni	(0.6)(0.3)(0.1)	(Al)(Cu)(Ni)
Al7Cu2Fe	(7)(2)(1)	(Al)(Cu)(Fe)

Name	Lattice Size	Constituent
Al7Cu4Ni	(7)(4)(1)	(Al)(Cu)(Ni)
AlCu2Ti	(0.75)(0.25)	(Al,Cu)(Ti)
AlCuTi	(0.6667)(0.3333)	(Al,Cu)(Ti)
AlLi2Zr	(0.25)(0.5)(0.25)	(Al)(Li)(Zr)
Co16Si7Ti6	(16)(7)(6)	(Co)(Si)(Ti)
Cr8Fe16Ti5	(0.828)(0.172)	(Cr,Fe)(Ti)
Cu2MgZr	(2)(1)(1)	(Cu)(Mg)(Zr)
Fe4V5Si4	(4)(5)(4)	(Fe)(V)(Si)
Fe5Ni3Si2	(0.8)(0.2)	(Fe,Ni)(Si)
Fe5V3Si2	(5)(3)(2)	(Fe)(V)(Si)
Mg2CrNi	(0.12)(0.33)(0.55)	(Cr,Ni)(Mg,Ni)(Cr,Mg)
Mg2SiNi3	(2)(1)(3)	(Mg)(Si)(Ni)
Ni11Si31Zr8	(0.22)(0.62)(0.16)	(Ni)(Si)(Zr)
Ni2Si9Zr14	(0.08)(0.36)(0.56)	(Ni)(Si)(Zr)
NiSnTi	(0.333)(0.333)(0.333)	(Ti)(Ni)(Sn)
NiTiZr	(1)(1)(1)	(Ni,Ti,Zr)(Ni,Ti,Zr)(Ni,Ti,Zr)

1.5 Assessed Subsystems

A total of **478** systems, including 203 binary and 275 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 (203)

Ag-Al(10)	Ag-B(10)	Ag-C(10)	Ag-Co(10)	Ag-Cr(10)	Ag-Cu(10)	Ag-Fe(10)
Ag-Mg(10)	Ag-Mn(10)	Ag-Mo(10)	Ag-Ni(10)	Ag-O(5)	Ag-Si(10)	Ag-Sn(10)
Ag-Ti(10)	Ag-V(10)	Ag-Zn(10)	Ag-Zr(10)	Al-B(10)	Al-C(10)	Al-Co(10)
Al-Cr(10)	Al-Cu(10)	Al-Fe(10)	Al-Hf(10)	Al-Li(10)	Al-Mg(10)	Al-Mn(10)
Al-Mo(10)	Al-Ni(10)	Al-O(10)	Al-Si(10)	Al-Sn(10)	Al-Ti(10)	Al-V(10)
Al-Zn(10)	Al-Zr(10)	B-C(10)	B-Co(10)	B-Cr(10)	B-Cu(10)	B-Fe(10)
B-Hf(10)	B-Mg(10)	B-Mn(10)	B-Mo(10)	B-Ni(10)	B-O(10)	B-Si(10)
B-Sn(10)	B-Ti(10)	B-V(10)	B-Zn(10)	B-Zr(10)	C-Co(10)	C-Cr(10)
C-Fe(10)	C-Hf(10)	C-Li(10)	C-Mg(10)	C-Mn(10)	C-Mo(10)	C-Ni(10)
C-O(10)	C-Si(10)	C-Sn(10)	C-Ti(10)	C-V(10)	C-Zn(10)	C-Zr(10)
Co-Cr(10)	Co-Cu(10)	Co-Fe(10)	Co-Hf(10)	Co-Li(10)	Co-Mg(10)	Co-Mn(10)
Co-Mo(10)	Co-Ni(10)	Co-O(10)	Co-Si(10)	Co-Sn(10)	Co-Ti(10)	Co-V(10)
Co-Zn(10)	Co-Zr(10)	Cr-Cu(10)	Cr-Fe(10)	Cr-Hf(10)	Cr-Li(10)	Cr-Mg(10)
Cr-Mn(10)	Cr-Mo(10)	Cr-Ni(10)	Cr-O(10)	Cr-Si(10)	Cr-Sn(10)	Cr-Ti(10)
Cr-V(10)	Cr-Zn(10)	Cr-Zr(10)	Cu-Fe(10)	Cu-Hf(10)	Cu-Li(10)	Cu-Mg(10)
Cu-Mn(10)	Cu-Mo(10)	Cu-Ni(10)	Cu-O(10)	Cu-Si(10)	Cu-Sn(10)	Cu-Ti(10)
Cu-V(10)	Cu-Zn(10)	Cu-Zr(10)	Fe-Hf(10)	Fe-Li(10)	Fe-Mg(10)	Fe-Mn(10)
Fe-Mo(10)	Fe-Ni(10)	Fe-O(10)	Fe-Si(10)	Fe-Sn(10)	Fe-Ti(10)	Fe-V(10)
Fe-Zn(10)	Fe-Zr(10)	Hf-Li(10)	Hf-Mg(10)	Hf-Mn(10)	Hf-Mo(10)	Hf-Ni(10)
Hf-O(10)	Hf-Si(10)	Hf-Sn(10)	Hf-Ti(10)	Hf-V(10)	Hf-Zr(10)	Li-Mg(10)
Li-Mn(10)	Li-Ni(10)	Li-O(10)	Li-Si(10)	Li-Sn(10)	Li-Ti(10)	Li-V(10)

Li-Zn(10) Li-Zr(10) Mg-Mn(10) Mg-Mo(10) Mg-Ni(10) Mg-O(10) Mg-Si(10)
Mg-Sn(10) Mg-Ti(10) Mg-V(10) Mg-Zn(10) Mg-Zr(10) Mn-Mo(10) Mn-Ni(10)
Mn-O(10) Mn-Si(10) Mn-Sn(10) Mn-Ti(10) Mn-V(10) Mn-Zn(10) Mn-Zr(10)
Mo-Ni(10) Mo-O(10) Mo-Si(10) Mo-Sn(10) Mo-Ti(10) Mo-V(10) Mo-Zr(10)
Ni-O(10) Ni-Si(10) Ni-Sn(10) Ni-Ti(10) Ni-V(10) Ni-Zn(10) Ni-Zr(10)
O-Si(10) O-Sn(10) O-Ti(10) O-V(10) O-Zn(5) O-Zr(10) Si-Sn(10)
Si-Ti(10) Si-V(10) Si-Zn(10) Si-Zr(10) Sn-Ti(10) Sn-V(10) Sn-Zn(10)
Sn-Zr(10) Ti-V(10) Ti-Zn(10) Ti-Zr(10) V-Zn(10) V-Zr(10) Zn-Zr(10)

Ternary Systems (275)

Ag-Al-Co(5) Ag-Al-Cu(10) Ag-Al-Fe(10) Ag-Al-Mg(10) Ag-Al-Si(10) Ag-Al-Sn(10)
Ag-Al-Zn(10) Ag-Co-Sn(5) Ag-Cr-Cu(10) Ag-Cu-Mg(10) Ag-Cu-Ni(10) Ag-Cu-Si(10)
Ag-Cu-Sn(10) Ag-Cu-Ti(10) Ag-Cu-Zr(10) Ag-Ni-Sn(10) Ag-Sn-Ti(5) Al-Co-Cr(10)
Al-Co-Cu(10) Al-Co-Fe(10) Al-Co-Mg(10) Al-Co-Mn(10) Al-Co-Mo(10) Al-Co-Ni(10)
Al-Co-Si(10) Al-Co-Ti(10) Al-Co-Zr(10) Al-Cr-Cu(10) Al-Cr-Fe(10) Al-Cr-Mg(10)
Al-Cr-Mn(10) Al-Cr-Mo(10) Al-Cr-Ni(10) Al-Cr-Si(10) Al-Cr-Ti(10) Al-Cr-Zr(10)
Al-Cu-Fe(10) Al-Cu-Li(10) Al-Cu-Mg(10) Al-Cu-Mn(10) Al-Cu-Mo(10) Al-Cu-Ni(10)
Al-Cu-Si(10) Al-Cu-Sn(10) Al-Cu-Ti(10) Al-Cu-V(10) Al-Cu-Zn(10) Al-Cu-Zr(10)
Al-Fe-Mg(8) Al-Fe-Mn(10) Al-Fe-Mo(8) Al-Fe-Ni(10) Al-Fe-Si(10) Al-Fe-Ti(10)
Al-Fe-V(10) Al-Fe-Zn(10) Al-Fe-Zr(10) Al-Li-Mg(10) Al-Li-Mn(10) Al-Li-Si(10)
Al-Li-Zr(10) Al-Mg-Mn(10) Al-Mg-Mo(8) Al-Mg-Si(10) Al-Mg-Sn(10) Al-Mg-Ti(10)
Al-Mg-Zn(10) Al-Mn-Ni(5) Al-Mn-Si(10) Al-Mn-Ti(10) Al-Mn-Zn(10) Al-Mo-Ni(10)
Al-Mo-Si(10) Al-Mo-Ti(10) Al-Mo-V(10) Al-Mo-Zr(10) Al-Ni-Si(10) Al-Ni-Ti(10)
Al-Ni-V(10) Al-Ni-Zn(10) Al-Ni-Zr(10) Al-Si-Sn(10) Al-Si-Ti(10) Al-Si-V(10)
Al-Si-Zn(10) Al-Si-Zr(10) Al-Sn-Ti(10) Al-Ti-V(10) Al-Ti-Zn(10) Al-Ti-Zr(10)
Al-V-Zr(10) C-Mo-Zr(10) Co-Cr-Cu(10) Co-Cr-Fe(10) Co-Cr-Mn(10) Co-Cr-Mo(10)
Co-Cr-Ni(10) Co-Cr-Si(10) Co-Cr-Ti(10) Co-Cr-V(10) Co-Cr-Zr(10) Co-Cu-Fe(10)
Co-Cu-Hf(10) Co-Cu-Mn(10) Co-Cu-Mo(10) Co-Cu-Ni(10) Co-Cu-Ti(10) Co-Fe-Mn(10)
Co-Fe-Mo(10) Co-Fe-Ni(10) Co-Fe-Si(10) Co-Fe-Ti(10) Co-Fe-V(10) Co-Fe-Zr(10)

Co-Hf-Zr(10)	Co-Mn-Mo(10)	Co-Mn-Ni(10)	Co-Mn-Si(10)	Co-Mn-Ti(10)	Co-Mn-Zr(10)
Co-Mo-Ni(10)	Co-Mo-Ti(10)	Co-Mo-Zr(10)	Co-Ni-Si(10)	Co-Ni-Ti(10)	Co-Ni-V(10)
Co-Si-Ti(10)	Co-Si-V(10)	Co-Si-Zr(10)	Co-Sn-Ti(10)	Co-V-Zr(10)	Cr-Cu-Fe(10)
Cr-Cu-Mn(10)	Cr-Cu-Mo(5)	Cr-Cu-Ni(10)	Cr-Cu-Sn(10)	Cr-Cu-Ti(10)	Cr-Cu-Zr(10)
Cr-Fe-Mg(10)	Cr-Fe-Mn(10)	Cr-Fe-Mo(10)	Cr-Fe-Ni(10)	Cr-Fe-Si(10)	Cr-Fe-Sn(10)
Cr-Fe-Ti(10)	Cr-Fe-V(10)	Cr-Fe-Zr(10)	Cr-Mg-Ni(10)	Cr-Mn-Ni(10)	Cr-Mn-Si(10)
Cr-Mn-Ti(10)	Cr-Mn-V(10)	Cr-Mn-Zr(10)	Cr-Mo-Ni(10)	Cr-Mo-Si(10)	Cr-Mo-Ti(10)
Cr-Mo-V(10)	Cr-Mo-Zr(10)	Cr-Ni-Si(10)	Cr-Ni-Ti(10)	Cr-Ni-V(10)	Cr-Ni-Zr(10)
Cr-Si-Ti(10)	Cr-Sn-Ti(10)	Cr-Sn-Zr(5)	Cr-Ti-V(10)	Cr-Ti-Zr(10)	Cr-V-Zr(10)
Cu-Fe-Mg(8)	Cu-Fe-Mn(10)	Cu-Fe-Mo(10)	Cu-Fe-Ni(10)	Cu-Fe-Si(10)	Cu-Fe-Sn(10)
Cu-Fe-Ti(10)	Cu-Fe-V(10)	Cu-Fe-Zn(8)	Cu-Fe-Zr(10)	Cu-Hf-Ni(10)	Cu-Mg-Mn(8)
Cu-Mg-Ni(10)	Cu-Mg-Si(10)	Cu-Mg-Sn(10)	Cu-Mg-Ti(10)	Cu-Mg-Zn(10)	Cu-Mg-Zr(10)
Cu-Mn-Ni(10)	Cu-Mn-Si(10)	Cu-Mn-Sn(10)	Cu-Mn-Ti(10)	Cu-Mn-Zn(10)	Cu-Ni-Si(10)
Cu-Ni-Sn(10)	Cu-Ni-Ti(10)	Cu-Ni-V(10)	Cu-Ni-Zr(10)	Cu-Si-Sn(10)	Cu-Si-Ti(10)
Cu-Si-Zn(10)	Cu-Sn-Ti(10)	Cu-Ti-Zr(10)	Fe-Mg-Mn(5)	Fe-Mg-Si(10)	Fe-Mg-Zn(5)
Fe-Mg-Zr(10)	Fe-Mn-Mo(10)	Fe-Mn-Ni(10)	Fe-Mn-Si(10)	Fe-Mn-Ti(10)	Fe-Mn-V(10)
Fe-Mn-Zn(5)	Fe-Mn-Zr(10)	Fe-Mo-Ni(10)	Fe-Mo-Si(5)	Fe-Mo-Ti(10)	Fe-Mo-V(10)
Fe-Mo-Zr(10)	Fe-Ni-Si(10)	Fe-Ni-Ti(10)	Fe-Ni-V(10)	Fe-Ni-Zn(10)	Fe-Ni-Zr(10)
Fe-Si-Sn(10)	Fe-Si-Ti(10)	Fe-Si-V(10)	Fe-Si-Zn(10)	Fe-Si-Zr(10)	Fe-Sn-Zr(10)
Fe-Ti-V(10)	Fe-Ti-Zn(10)	Fe-Ti-Zr(10)	Hf-Ni-Ti(10)	Hf-Ni-Zr(5)	Hf-Ti-Zr(10)
Li-Mg-Si(10)	Li-Mg-Zr(10)	Mg-Mn-Ni(10)	Mg-Mn-Si(10)	Mg-Mn-Zn(8)	Mg-Ni-Si(10)
Mg-Ni-Zn(10)	Mg-Si-Sn(10)	Mg-Si-Zn(10)	Mg-Si-Zr(10)	Mn-Mo-Ni(10)	Mn-Mo-Ti(10)
Mn-Ni-Si(10)	Mn-Ni-Ti(10)	Mn-Si-Sn(10)	Mn-Si-Ti(10)	Mn-Si-Zn(5)	Mn-Ti-V(10)
Mn-Ti-Zr(10)	Mo-Ni-Si(10)	Mo-Ni-Ti(10)	Mo-Ni-V(10)	Mo-Ni-Zr(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)	Ni-Si-Ti(10)
Ni-Si-V(10)	Ni-Si-Zn(10)	Ni-Si-Zr(10)	Ni-Sn-Ti(10)	Ni-Sn-Zr(10)	Ni-Ti-V(10)
Ni-Ti-Zr(10)	Ni-V-Zr(10)	Si-Ti-V(10)	Sn-Ti-Zr(10)	Ti-V-Zr(10)	

1.6 Database Applications

The PanHEA database is validated by a large amount of experimental data. It is by far the most comprehensive database for alloy design and processing optimization of high entropy alloys for 3rd-transition metals. A few example calculations using the current PanHEA database are given below:

Figure 1.1 shows the calculated isopleth of the $Al_xCoCrFeNi$ system with x varies between 0~2. x is the Al ratio and other elements are in the equal atomic percent. It indicates that Al is a strong stabilizer for both the disorder Bcc and ordered B2 structure, and the later is favored. In addition to the phase equilibrium information with the changing of Al ratio at different temperatures, one can also predict the as-cast microstructures of the HEAs based on the calculated mushy-zone (Liquid + Solid) phase regions (as indicated on top of this figure). It shows that pure Fcc structure will be developed with lower Al ratio, while Bcc structure (Bcc and/or B2) will be developed with higher Al ratio, and a mixture of Fcc+Bcc should be seen in between. Our predictions are exactly what were observed by many researchers who have carried our experimental studies of $Al_xCoCrFeNi$ alloys [2006Ke, 2008Wan, 2011Kao].

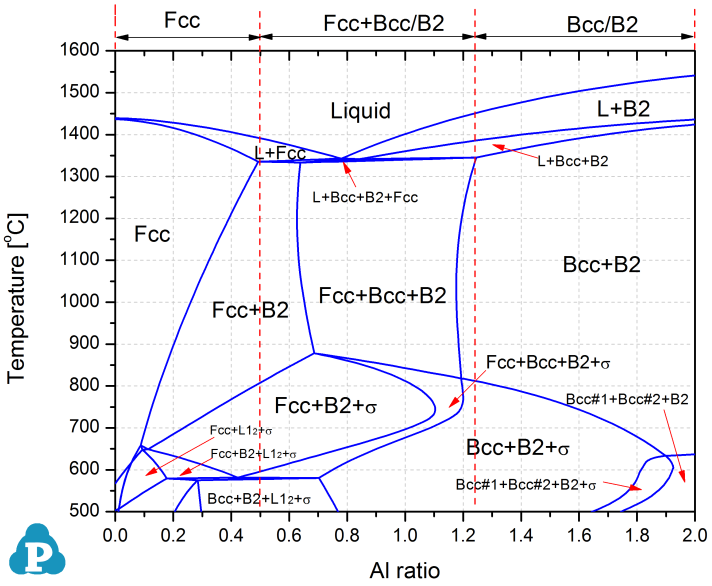


Figure 1.1: Calculated isopleth of the $Al_xCoCrFeNi$ with x=0~2

For quantitative analysis on the phase transformations of an alloy at the given composition, the equilibrium calculation is needed. Figure 1.2 shows equilibrium calculation of the $Al_{0.3}CoCrFeNi$ alloy at the temperature range from 600 to 1450 °C. It indicates that this alloy contains single Fcc phase at higher temperatures (>1000 °C). The B2 phase precipitates out at around 1000 °C. At lower temperatures (<700 °C), other phases will form as well, such as σ and L12_Fcc. The alloy with Fcc structure shows good ductility but low strength, while the B2-type intermetallic compounds generally show excellent strength but low ductility. Usually, an HEA with dispersed B2 precipitates within the Fcc matrix has balanced properties and good performance. On the basis of thermodynamic calculations (as shown in Figure 1.2), the $Al_{0.3}CoCrFeNi$ HEA may meet the requirements. As shown in Figure 1.2, the solvus temperature of B2 is about 1060 °C. When annealing below this temperature, the B2 precipitates will form. Shu et al. [2009Shu] investigated the microstructure and tensile behaviors of the $Al_{0.3}CoCrFeNi$ HEA, and they found that the as-cast structure of this alloy is Fcc and the B2 phase formed when aged at 900 °C for 72h. The tensile strength of this alloy after heat treatment was significantly improved. Prediction from our database agrees with their experimental observation very well.

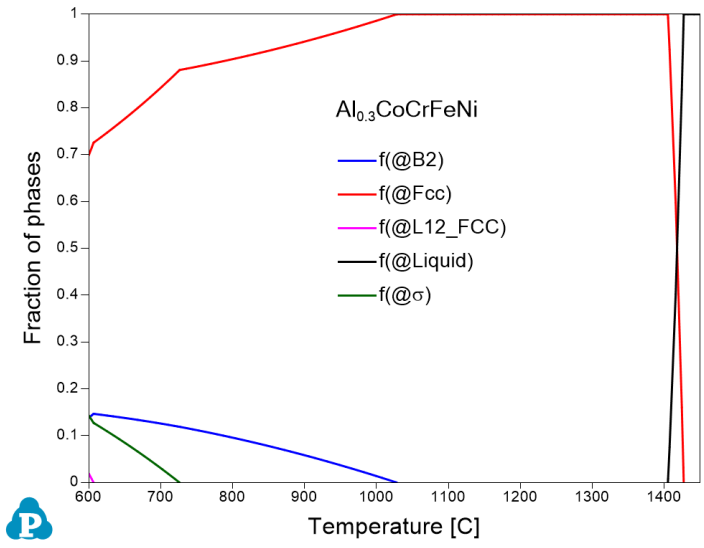


Figure 1.2: Equilibrium calculation of $Al_{0.3}CoCrFeNi$ HEA

2 Mobility Database

PanHEA2024_MB is an atomic mobility database for high entropy alloys (HEA), which is compatible with the `PanHEA2024_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

	Ag	Al	Co	Cr	Cu	Fe	Hf	Li	Mg	Mn	Mo	Ni	Si	Sn	Ti	V	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 PanHEA2024_MB database are also assessed. In the following, the assessed chemical-diffusivity within the binary and ternary systems for the Bcc, Fcc, and Hcp phases are listed, respectively.

Fcc Phase

Ag-Al	Ag-Cu	Ag-Sn	Al-Co	Al-Cu	Al-Mg	Al-Ni	Al-Si	Co-Cr	Co-Cu
Co-Fe	Co-Ni	Cr-Fe	Cr-Ni	Cu-Fe	Cu-Mg	Cu-Si	Cu-Sn	Cu-Ti	Fe-Mn
Fe-Ni	Fe-Si	Mn-Ni	Ni-Ti	Ni-V					

Al-Co-W	Al-Cr-Ni	Al-Cu-Mg	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	Cu-Ti	Fe-Ti	Ti-V	Ti-Zr		
Al-Cr-Ti	Al-Fe-Ti	Cr-Fe-Ni							

Hcp Phase

Al-Mg		

2.4 Database Validation

The simulated concentration profiles of a series of high entropy alloys are shown below to validate the current PanHEA2024_MB database.

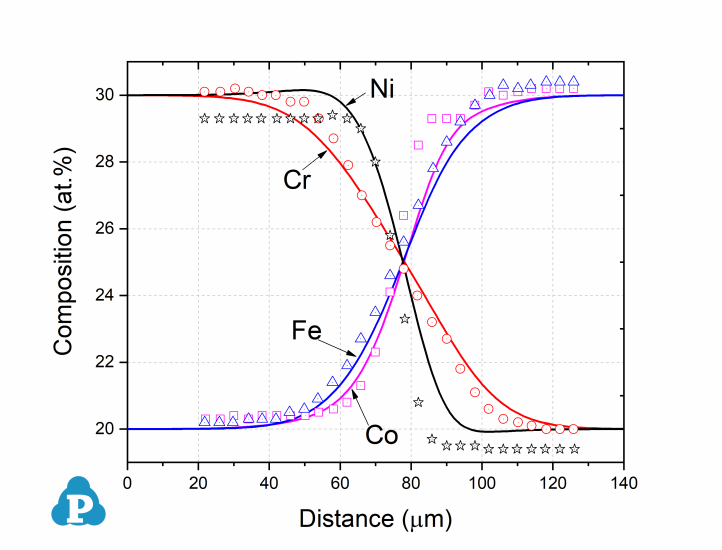


Figure 2.1: Simulated concentration profiles of Co-30Cr-20Fe-30Ni/Co-20Cr-30Fe-20Ni (at.%) diffusion couple annealed at 1000 °C for 100h with experimental data (symbols) of ref. [2015Kul]

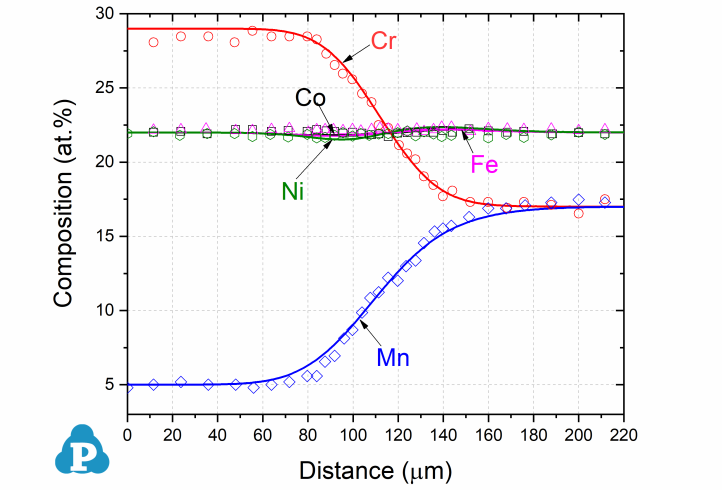


Figure 2.2: Simulated concentration profiles of Co22Cr29Fe22Mn5Ni22/Co22Cr17Fe22Mn17Ni22 (at.%) diffusion couple annealed at 1000 °C for 100h with experimental data (symbols) from ref. [2013Tsa]

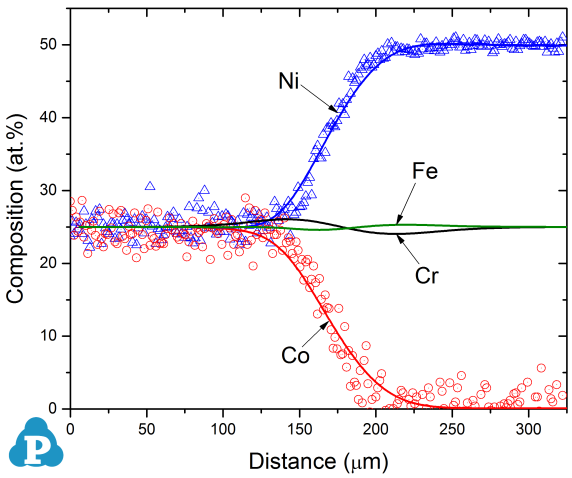


Figure 2.3: Simulated concentration profiles of Co25Cr25Fe25Ni25/Ni50Cr25Fe25 (at.%) diffusion couple annealed at 1120 °C for 48h with experimental data (symbols) of ref. [2017Zha]

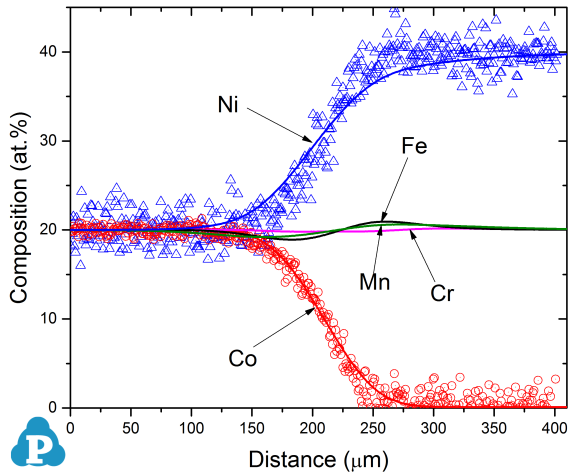


Figure 2.4: Simulated concentration profiles of Co20Cr20Fe20Mn20Ni20/ Cr20Fe20Mn20Ni40 (at.%) diffusion couple annealed at 1070 °C for 94.5 h with experimental data (symbols) of ref. [2017Zha]

3 Thermophysical Property Database

The thermophysical property database **PanHEA2024_ TP** is compatible with the `PanHEA2024_ TH` thermodynamic database and suitable for the simulation of thermophysical properties of high entropy 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 **687** phases assessed in the `PanHEA2024_ TH` database. It is used to calculate the density, thermal expansion, solidification shrinkage of high entropy alloys (HEA).

Figure 3.1 shows the calculated linear thermal expansion coefficients (CTE) for alloys with equiatomic ratio in the Co-Cr-Fe-Ni system (binary CoNi, ternary CoCrNi, CoFeNi, CrFeNi, and quaternary CoCrFeNi), which are in good agreement with the experimental measurements in the literature [2018Lap]. Figure 3.2 shows calculated density contour mapping of the Co-Cr-Fe-20Mn-20Ni (at.%) at 1000 °C. One can see that the stable phase regions include Fcc single phase field and Bcc+Fcc two-phase field in this isothermal section. The density of these HEAs at 1000 °C will vary between 7.2~7.9 g/cm3.

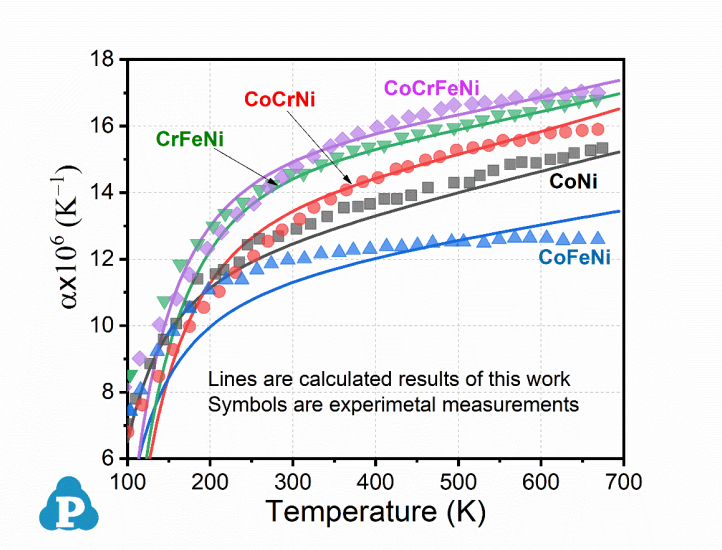


Figure 3.1: Calculated linear thermal expansion coefficient of the HEAs within the Co-Cr-Fe-Mn-Ni system with experimental data from ref. [2018Lap]

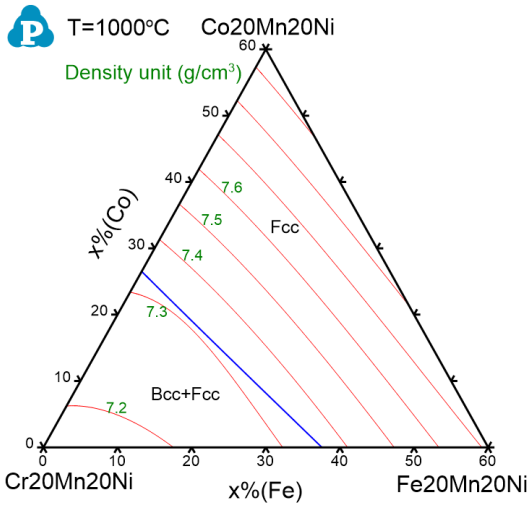


Figure 3.2: Density contour mapping of Co-Cr-Fe-20Mn-20Ni (at.%) at 1000 °C

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 CoCrFeMnNi high entropy alloy.

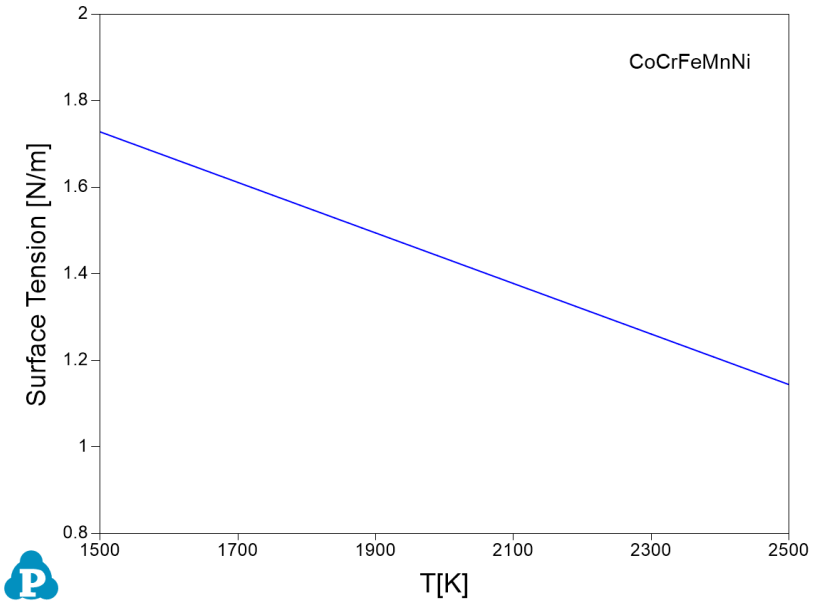


Figure 3.3: Surface tension of CoCrFeMnNi high entropy alloy

3.3 Viscosity

The viscosity of the liquid phase is added into the property database. Figure 3.4 shows the viscosity of CoCrFeMnNi high entropy alloy.

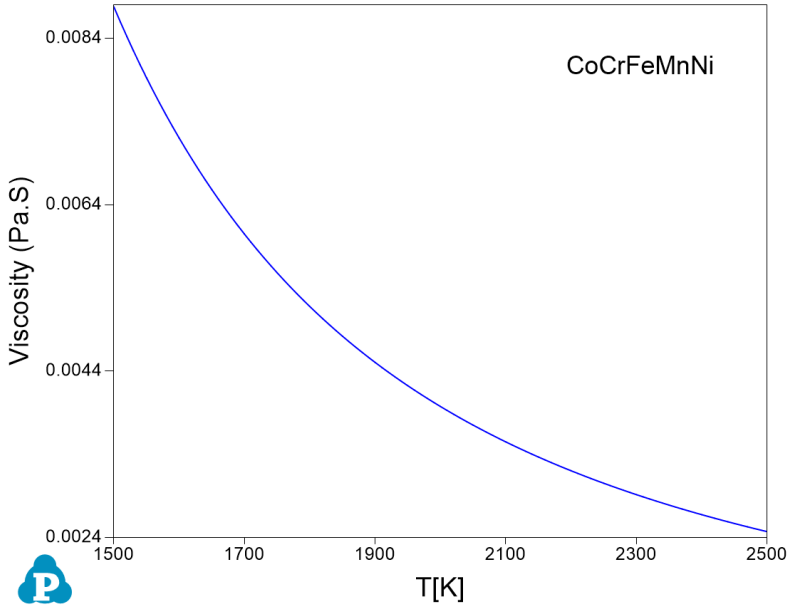


Figure 3.4: Viscosity of the CoCrFeMnNi high entropy alloy

4 References

[2006Ke] G.Y. Ke, S.K. Chen, T. Hsu, J.W. Yeh, Annales de Chimie- Science Des Matériaux, 31(6) (2006): 669-684.

[2008Wan] Y.P. Wang, B.S. Li, M.X. Ren, C. Yang, H.Z. Fu, Mat. Sci. Eng. A, 491(1-2) (2008): 154-158.

[2009Shu] T.T. Shun, Y.C. Du, J Alloys Compd., 479 (2009): 157-160.

[2011Kao] Y.F. Kao, S.K. Chen, T.J. Chen, P.C. Chu, J.W. Yeh,, S.J. Lin, J Alloys Compd., 509 (2011): 1607-1614.

[2013Tsa] K.-Y. Tsai, M.-H. Tsai and J.-W. Yeh, Sluggish diffusion in Co-Cr-Fe–Mn-Ni high-entropy alloys. Acta Materialia, 61(13) (2013): 4887-4897.

[2015Kul] K. Kulkarni and G.P.S. Chauhan, Investigations of quaternary interdiffusion in a constituent system of high entropy alloys. AIP Advances, (6) 2015: 097162.

[2017Zha] C. Zhang, et al., Understanding of the Elemental Diffusion Behavior in Concentrated Solid Solution Alloys. J. Phase Equilib. Diffus., 38 (2017): 434-444.

PanHEA2024: List of Phases

Phases (**687**)

Name	Model	Lattice Size	Constituent
A15	CEF (SLN)	(0.75)(0.25) (0.05)	(Cr,Fe,Mo,Si,Ti,V,Zr) (Al,Cr,Ni,Si,Ti,V)(Va)
A3B	CEF (SLN)	(3)(1)	(Co,Cr,Fe,Mo,Si,V)(Al,Cr,Mo,Si,V)
ALPHA_ RHOMBO_B	CEF (ST1)	(1)	(B)
A_Co59Si26V15	CEF (ST3)	(0.59)(0.26) (0.15)	(Co)(Si)(V)
A_Li2Zn3	CEF (SLN)	(2)(3)	(Li)(Li,Zn)
A_Li2Zn5	CEF (SLN)	(2)(5)	(Li,Zn)(Zn)
A_LiZn4	CEF (SLN)	(1)(4)	(Li,Zn)(Li,Zn)
A_TiO	CEF (ST2)	(1)(1)	(Ti)(O)
Ag14Cu70Zr16	CEF (ST3)	(0.14)(0.7) (0.16)	(Ag)(Cu)(Zr)
Ag2O2	CEF (ST2)	(2)(2)	(Ag)(O)
Ag3Sn	CEF (SLN)	(0.75)(0.25)	(Ag)(Ag,Sn)
Ag5Zn8	CEF (SLN)	(2)(2)(3)(6)	(Ag,Zn)(Ag)(Ag,Zn)(Ag,Zn)
AgMg3	CEF (SLN)	(0.23)(0.77)	(Ag,Cu)(Al,Mg)
AgMg4	CEF (SLN)	(0.2)(0.8)	(Ag,Cu)(Al,Mg)
AgZn2	CEF (SLN)	(1)(2)	(Zn)(Ag,Zn)
AgZn3	CEF (SLN)	(1)	(Ag,Zn)
AgZr	CEF (SLN)	(0.5)(0.5)	(Ag,Cu)(Zr)

Name	Model	Lattice Size	Constituent
Al10Cu10Fe	CEF (ST3)	(10)(10)(1)	(Al)(Cu)(Fe)
Al10Fe3Ni	CEF (ST3)	(10)(3)(1)	(Al)(Fe)(Ni)
Al10FeNi3	CEF (ST3)	(10)(1)(3)	(Al)(Fe)(Ni)
Al10V	CEF (SLN)	(10)(1)	(Al)(Fe,Mo,V)
Al114Cu65Mn21	CEF (ST3)	(114)(65)(21)	(Al)(Cu)(Mn)
Al11Co6Si6	CEF (ST3)	(11)(6)(6)	(Al)(Co)(Si)
Al11Cr2	CEF (SLN)	(10)(1)(2)	(Al)(Al)(Cr,Mn)
Al11Mn4_H	CEF (SLN)	(29)(10)	(Al,Cu,Mn)(Cu,Mn)
Al11Mn4_L	CEF (SLN)	(11)(4)	(Al,Zn)(Cr,Mn)
Al12Fe7Mo	CEF (ST3)	(0.45)(0.4) (0.15)	(Al)(Fe)(Mo)
Al12Mn	CEF (ST2)	(12)(1)	(Al)(Mn)
Al12Mo	CEF (SLN)	(12)(1)	(Al)(Mo,V)
Al12_Fe3V3Si	CEF (SLN)	(12)(3)(1)	(Al)(Fe,V)(Si)
Al13Cr2	CEF (ST2)	(13)(2)	(Al)(Cr)
Al13Cu4Mn3	CEF (ST3)	(13)(4)(3)	(Al)(Cu)(Mn)
Al13M4	CEF (SLN)	(0.6275) (0.235) (0.1375)	(Al,Cu)(Co,Cr,Fe,Mn,Ni,Si,V,Zn) (Al,Si,Zn,Va)
Al14Mn4Si5	CEF (SLN)	(14)(4)(5)	(Al)(Mn)(Al,Si)
Al15_FeMn3Si2	CEF (SLN)	(16)(4)(1)(2)	(Al)(Fe,Mn)(Si)(Al,Si)
Al16Co7Zr6	CEF (ST3)	(16)(7)(6)	(Al)(Co)(Zr)
Al17Cr2Mg4	CEF (SLN)	(21)(2)	(Al,Mg)(Cr)
Al17Mo4	CEF (SLN)	(17)(4)	(Al)(Mo,V)
Al18Mg3Mo2	CEF (ST3)	(18)(3)(2)	(Al)(Mg)(Mo)

Name	Model	Lattice Size	Constituent
Al18Mg3X2	CEF (SLN)	(18)(3)(2)	(Al)(Mg)(Mn,Ti,V)
Al1Fe1O3	CEF (ST3)	(1)(1)(3)	(Al+3)(Fe+3)(O-2)
Al22Mo5	CEF (SLN)	(22)(5)	(Al)(Mo,V)
Al23V4	CEF (SLN)	(23)(4)	(Al,Cu,Si)(Fe,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,Cu,Si,Zn)(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)
Al2Li3	CEF (ST2)	(2)(3)	(Al)(Li)
Al2LiMg	CEF (ST3)	(0.53)(0.33) (0.14)	(Al)(Li)(Mg)
Al2Mn2Si3	CEF (ST3)	(2)(2)(3)	(Al)(Mn)(Si)
Al2MnSi3	CEF (ST3)	(2)(1)(3)	(Al)(Mn)(Si)
Al2Ti	CEF (SLN)	(2)(1)	(Al,Cr,Ti)(Al,Ti,Zr)
Al2Zr	CEF (ST2)	(2)(1)	(Al)(Zr)
Al2Zr3	CEF (SLN)	(2)(3)	(Al)(Ti,V,Zr)
Al31Mn8Zn11	CEF (ST3)	(0.62)(0.16) (0.22)	(Al)(Mn)(Zn)
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)
Al3Cu5Zn2	CEF (SLN)	(1)(4)(4)(1)	(Al,Cu)(Al)(Cu)(Zn)

Name	Model	Lattice Size	Constituent
Al3Hf2	CEF (SLN)	(0.6)(0.4)	(Al,Si)(Hf)
Al3Hf4	CEF (SLN)	(0.42857) (0.57143)	(Al,Si)(Hf)
Al3Hf_alpha	CEF (SLN)	(0.75)(0.25)	(Al,Si)(Hf)
Al3Hf_beta	CEF (SLN)	(0.75)(0.25)	(Al,Si)(Hf)
Al3Li8Si5	CEF (ST3)	(8)(3)(5)	(Li)(Al)(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)(Mo,V)
Al3Ni	CEF (SLN)	(0.75)(0.25)	(Al)(Ni,V)
Al3Ni5	CEF (ST2)	(0.375)(0.625)	(Al)(Ni)
Al3Ni8Zn9	CEF (ST3)	(3)(8)(9)	(Al)(Ni)(Zn)
Al3NiM2	CEF (SLN)	(3)(2)(1)	(Al,Si)(Al,Co,Cu,Ni,V,Zr)(Co,Cu,Ni,Va)
Al3V	CEF (SLN)	(3)(1)	(Al,Cu,Ni,Si)(Fe,Mo,V,Zr)
Al3Zr	CEF (SLN)	(3)(1)	(Al,Li,Si)(Ti,V,Zr)
Al3Zr2	CEF (SLN)	(3)(2)	(Al,Li)(Zr)
Al3Zr4	CEF (SLN)	(3)(4)	(Al,Cu,Li)(Zr)
Al3Zr5	CEF (SLN)	(3)(5)	(Al)(Li,V,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)(C)
Al4CoZr	CEF (ST3)	(4)(1)(1)	(Al)(Co)(Zr)
Al4Cr	CEF (SLN)	(4)(1)	(Al,Si)(Cr)
Al4Li9	CEF (ST2)	(4)(9)	(Al)(Li)
Al4Mn4Si2	CEF (SLN)	(0.8)(0.2)	(Al,Mn)(Si)

Name	Model	Lattice Size	Constituent
Al4Mn_R	CEF (ST2)	(461)(107)	(Al)(Mn)
Al4Mn_U	CEF (SLN)	(0.2)(0.8)	(Cr,Fe,Mn)(Al,Li,Zn,Va)
Al4Mo	CEF (SLN)	(4)(1)	(Al)(Mo,V)
Al4Zr5	CEF (ST2)	(4)(5)	(Al)(Zr)
Al5Co2	CEF (SLN)	(5)(2)	(Al,Si)(Co,Fe)
Al5CoCu4	CEF (ST3)	(5)(1)(4)	(Al)(Co)(Cu)
Al5CuTi2	CEF (SLN)	(0.75)(0.25)	(Al,Cu)(Ti)
Al5Fe2	CEF (SLN)	(5)(2)(3)	(Al,Cu,Si)(Co,Cr,Fe,Mn,Ni,V)(Zn,Va)
Al5Fe4	CEF (SLN)	(1)	(Al,Fe,Mn)
Al5Mn2Si5	CEF (ST3)	(0.7)(0.2)(0.1)	(Al)(Mn)(Si)
Al5Mn6Si7	CEF (ST3)	(5)(6)(7)	(Al)(Mn)(Si)
Al5Mo	CEF (SLN)	(5)(1)	(Al)(Mo,V)
Al5Ti2	CEF (SLN)	(5)(2)	(Al,Ti)(Al,Mo,Ti)
Al5Ti3	CEF (ST2)	(5)(3)	(Al)(Ti)
Al60Cu4Mn11	CEF (ST3)	(0.8)(0.05) (0.15)	(Al)(Cu)(Mn)
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)
Al6CoCu3	CEF (ST3)	(6)(1)(3)	(Al)(Co)(Cu)
Al6Cu2Fe	CEF (SLN)	(0.62)(0.255) (0.125)	(Al)(Al,Cu)(Fe)
Al6Cu3Ni	CEF (ST3)	(0.6)(0.3)(0.1)	(Al)(Cu)(Ni)
Al6Mn	CEF (SLN)	(6)(1)	(Al,Li)(Mn)
Al6MoZr	CEF (ST3)	(6)(1)(1)	(Al)(Mo)(Zr)

Name	Model	Lattice Size	Constituent
Al6Ni3Si	CEF (ST3)	(6)(3)(1)	(Al)(Ni)(Si)
Al71Mn16Zn13	CEF (ST3)	(0.71)(0.16) (0.13)	(Al)(Mn)(Zn)
Al7Co4Si2	CEF (ST3)	(7)(4)(2)	(Al)(Co)(Si)
Al7CoCu2	CEF (ST3)	(7)(1)(2)	(Al)(Co)(Cu)
Al7Cu2Fe	CEF (ST3)	(7)(2)(1)	(Al)(Cu)(Fe)
Al7Cu4Ni	CEF (ST3)	(7)(4)(1)	(Al)(Cu)(Ni)
Al7V	CEF (SLN)	(7)(1)	(Al,Cu,Si)(Fe,Mo,V)
Al7VZr2	CEF (ST3)	(7)(1)(2)	(Al)(V)(Zr)
Al8Cr5_H	CEF (SLN)	(8)(5)	(Al)(Cr,Ti)
Al8Cr5_L	CEF (SLN)	(8)(5)	(Al,Si)(Cr,Fe,Ti)
Al8FeMg3Si6	CEF (ST4)	(8)(3)(1)(6)	(Al)(Mg)(Fe)(Si)
Al8FeMnSi2	CEF (ST4)	(16)(2)(2)(3)	(Al)(Fe)(Mn)(Si)
Al8Mn5	CEF (SLN)	(0.4615) (0.1923) (0.3462)	(Al)(Cu,Fe,Mn)(Al,Cu,Fe,Mn,Si,Ti,Zn)
Al8Mo3	CEF (SLN)	(8)(3)	(Al,Ti)(Mo,V)
Al8V5	CEF (SLN)	(8)(5)	(Al,Cu,Si)(Fe,Mo,Ni,Ti,V,Zr)
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	CEF (ST2)	(1)(12)	(Al)(B)
AlCo2Zr	CEF (ST3)	(1)(2)(1)	(Al)(Co)(Zr)
AlCr2	CEF (SLN)	(1)(2)	(Al,Si)(Cr)

Name	Model	Lattice Size	Constituent
AlCu2Ti	CEF (SLN)	(0.75)(0.25)	(Al,Cu)(Ti)
AlCuTi	CEF (SLN)	(0.6667) (0.3333)	(Al,Cu)(Ti)
AlCu_Delta	CEF (ST2)	(0.4)(0.6)	(Al)(Cu)
AlCu_Eps	CEF (SLN)	(0.5)(0.5)	(Al,Cu)(Cu,V)
AlCu_Eta	CEF (SLN)	(0.5)(0.5)	(Al,Cu)(Cu,V)
AlCu_Gamma	CEF (SLN)	(1)(1)	(Al,Cu,Mn,Si)(Va)
AlCu_Theta	CEF (SLN)	(0.667)(0.333)	(Al)(Al,Cu,Ti,V,Zr)
AlCu_Zeta	CEF (ST2)	(0.45)(0.55)	(Al)(Cu)
AlFeTi_T1	CEF (ST3)	(0.25)(0.5) (0.25)	(Al)(Fe)(Ti)
AlFeTi_T2	CEF (ST3)	(0.53448) (0.25172) (0.2138)	(Al)(Fe)(Ti)
AlFeTi_T3	CEF (ST3)	(0.65)(0.075) (0.275)	(Al)(Fe)(Ti)
AlFeTi_T4	CEF (ST3)	(0.35)(0.23) (0.42)	(Al)(Fe)(Ti)
AlHf	CEF (SLN)	(0.5)(0.5)	(Al,Si)(Hf)
AlLi2Zr	CEF (ST3)	(0.25)(0.5) (0.25)	(Al)(Li)(Zr)
AlLi5Si2	CEF (ST3)	(5.3)(0.7)(2)	(Li)(Al)(Si)
AlLiSi	CEF (ST3)	(1)(1)(1)	(Li)(Al)(Si)
AlMg_Beta	CEF (SLN)	(89)(140)	(Mg,Li)(Al,Cu,Zn)
AlMg_Eps	CEF (SLN)	(23)(30)	(Mg)(Al,Cu,Zn)
AlMg_Gamma	CEF (SLN)	(10)(24)(24)	(Mg)(Al,Cu,Li,Mg,Zn)(Al,Cu,Mg,Zn)

Name	Model	Lattice Size	Constituent
AlMnSi	CEF (ST3)	(1)(1)(1)	(Al)(Mn)(Si)
AlMoSi_C40	CEF (SLN)	(2)(1)	(Al,Si)(Mo)
AlMoSi_C54	CEF (ST3)	(0.434)(0.333)(0.233)	(Al)(Mo)(Si)
AlNi16Si9	CEF (ST3)	(1)(16)(9)	(Al)(Ni)(Si)
AlNi2Si	CEF (SLN)	(1)(1)	(Ni)(Al,Si,Va)
AlNi2Zn	CEF (ST3)	(1)(2)(1)	(Al)(Ni)(Zn)
AlNiTi_T1	CEF (ST3)	(0.65)(0.1)(0.25)	(Al)(Ni)(Ti)
AlNiTi_T2	CEF (SLN)	(0.5517)(0.2069)(0.2414)	(Al,Ti)(Ti)(Ni)
AlZr	CEF (SLN)	(1)(1)	(Al,Li)(Zr)
AlZr2	CEF (SLN)	(1)(2)	(Al)(V,Zr)
AlZr3	CEF (ST2)	(1)(3)	(Al)(Zr)
Alpha-Mn2B	CEF (ST2)	(0.670691)(0.329309)	(Mn)(B)
Alpha_AlFeSi	CEF (SLN)	(0.66)(0.19)(0.05)(0.1)	(Al)(Fe,V)(Si)(Al,Si)
Alpha_Co2Si	CEF (SLN)	(2)(1)	(Co,Cr,Fe,Mn,Si,Ti,Zr)(Co,Si)
Alpha_Cr5Si3	CEF (SLN)	(5)(3)	(Cr,Fe)(Si)
Alpha_TiMn	CEF (SLN)	(1)(1)	(Cr,Mn)(Ti)
B11	CEF (SLN)	(0.5)(0.5)	(Ag,Cu,Ni,Ti)(Ag,Cu,Ni,Ti)
B2	CEF (SLN)	(1)(1)	(Al,Co,Cr,Cu,Fe,Hf,Mn,Mo,Ni,Si,Ti,V,Zn,Zr)(Co,Cr,Cu,Fe,Hf,Mn,Mo,Ni,Si,Sn,Ti,V,Zr,Va)

Name	Model	Lattice Size	Constituent
B2O3	CEF (ST2)	(2)(3)	(B)(O)
B32	CEF (SLN)	(0.5)(0.5)(3)	(Al,Cu,Li,Mg,Mn,Zn) (Al,Cu,Li,Mg,Mn,Zn)(Va)
B4C	CEF (SLN)	(1)(1)	(B12,B11C)(B2,B2C,BC2)
B4Hf3	CEF (ST2)	(4)(3)	(B)(Hf)
BCT_A5	CEF (SLN)	(1)	(Ag,Al,Cu,Ni,Sn,Ti,Zn)
BETA_RHOMBO_B	CEF (SLN)	(93)(12)	(B)(B,Cu,Mn,Si,Zr)
BETA_VO	CEF (SLN)	(1)(1)	(V)(O,Va)
BHf	CEF (ST2)	(1)(1)	(B)(Hf)
BRONZE	CEF (SLN)	(2)(5)(1)	(V+4,V+5)(O-2)(Va)
B_Co27Si27V46	CEF (ST3)	(0.27)(0.27) (0.46)	(Co)(Si)(V)
B_Li2Zn3	CEF (SLN)	(2)(3)	(Li,Zn)(Li,Zn)
B_Li2Zn5	CEF (SLN)	(2)(5)	(Li,Zn)(Zn)
B_LiZn4	CEF (SLN)	(0.2)(0.8)(0.5)	(Li,Zn)(Li,Zn)(Va)
Bcc	CEF (SLN)	(1)(3)	(Ag,Al,Co,Cr,Cu,Fe,Hf,Li,Mg,Mn,Mo, Ni,Si,Sn,Ti,V,Zn,Zr)(B,C,O,Va)
Bcc_B2	CEF (SLN)	(0.5)(0.5)(3)	(Ag,Al,Co,Cr,Cu,Fe,Mg,Mn,Ni,Si,Ti,V) (Ag,Al,Co,Cr,Cu,Fe,Mg,Mn,Ni,Si,Ti,V) (Va)
Beta_AlFeSi	CEF (SLN)	(0.598)(0.152) (0.1)(0.15)	(Al)(Fe,Mn,V)(Si)(Al,Si)
Beta_Co2Si	CEF (SLN)	(2)(1)	(Co,Si)(Co,Si)
Beta_TiMn	CEF (SLN)	(0.515)(0.485)	(Cr,Mn,V)(Ti,Zr)
CBCC_A12	CEF (SLN)	(1)(1)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Ni,Si,Sn,Ti,

Name	Model	Lattice Size	Constituent
			V,Zn,Zr)(C,Va)
CHI_A12	CEF (SLN)	(24)(10)(24)	(Co,Cr,Fe,Ni)(Cr,Mo,Ti,Zr) (Co,Cr,Fe,Mo,Ni)
CUB_A13	CEF (SLN)	(1)(1)	(Ag,Al,Co,Cr,Cu,Fe,Hf,Mg,Mo,Mn,Ni, Si,Sn,Ti,V,Zn,Zr)(C,Va)
C_Co34Si27V39	CEF (ST3)	(0.34)(0.27) (0.39)	(Co)(Si)(V)
Cementite	CEF (SLN)	(3)(1)	(Co,Cr,Fe,Mn,Mo,Ni,V)(C)
Co10Cu57Ti33	CEF (ST3)	(0.57)(0.1) (0.33)	(Cu)(Co)(Ti)
Co16Si7Ti6	CEF (ST3)	(16)(7)(6)	(Co)(Si)(Ti)
Co2Mg	CEF (ST2)	(2)(1)	(Co)(Mg)
Co2Si13Ti5	CEF (ST3)	(2)(13)(5)	(Co)(Si)(Ti)
Co2SiTi	CEF (ST3)	(2)(1)(1)	(Co)(Si)(Ti)
Co2SnTi	CEF (SLN)	(1)(1)(1)(1)	(Co,Va)(Co)(Sn)(Ti)
Co3B	CEF (SLN)	(3)(1)	(Co,Fe)(B)
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)
Co3Sn2	CEF (SLN)	(1)(1)(0.5) (0.5)	(Co)(Sn)(Co,Va)(Co,Va)
Co3V	CEF (SLN)	(0.75)(0.25)	(Co,Cr,Fe,V)(Co,Cr,Fe,V)
Co4Zn	CEF (SLN)	(1)(1)	(Co,Zn)(Va)
Co5Cr5Si6	CEF (ST3)	(5)(5)(6)	(Co)(Cr)(Si)

Name	Model	Lattice Size	Constituent
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,Ti)(Co,Ni,Ti)
CoSi2Ti	CEF (ST3)	(1)(2)(1)	(Co)(Si)(Ti)
CoSiTi	CEF (ST3)	(1)(1)(1)	(Co)(Si)(Ti)
CoSn	CEF (ST2)	(0.5)(0.5)	(Co)(Sn)
CoSn2	CEF (ST2)	(0.333)(0.667)	(Co)(Sn)
CoSn3	CEF (ST2)	(0.25)(0.75)	(Co)(Sn)
CoSnTi	CEF (ST3)	(1)(1)(1)	(Co)(Sn)(Ti)
CoV3	CEF (SLN)	(1)(3)	(Co,Fe)(Cr,V)
CoZn14	CEF (ST2)	(0.0714286) (0.928571)	(Co)(Zn)
CoZn7	CEF (ST2)	(0.125)(0.875)	(Co)(Zn)
CoZn_Beta	CEF (SLN)	(1)(1)	(Co,Zn)(Va)
CoZn_Delta	CEF (ST2)	(0.117647) (0.882353)	(Co)(Zn)
CoZr3	CEF (ST2)	(1)(3)	(Co)(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)
Cr3B4	CEF (ST2)	(0.429)(0.571)	(Cr)(B)
Cr3Mn5	CEF (ST2)	(3)(5)	(Cr)(Mn)
Cr3Si	CEF (SLN)	(3)(1)	(Co,Cr,Mn,Ni,Si)(Al,Co,Cr,Si)
Cr5B3	CEF (ST2)	(0.625)(0.375)	(Cr)(B)
CrB4	CEF (ST2)	(0.2)(0.8)	(Cr)(B)
CrNiV	CEF (SLN)	(0.65)(0.35)	(Cr,V)(Ni)

Name	Model	Lattice Size	Constituent
CrSi2	CEF (SLN)	(1)(2)	(Cr,Si,Mo)(Al,Cr,Si)
CrZn17	CEF (ST2)	(0.05556) (0.94444)	(Cr)(Zn)
Cristobalite	CEF (ST2)	(1)(2)	(Si)(O)
Cu10Sn3	CEF (SLN)	(1)	(Cu,Sn)
Cu28Mn61Si11	CEF (ST3)	(0.28)(0.61) (0.11)	(Cu)(Mn)(Si)
Cu2MgZr	CEF (ST3)	(2)(1)(1)	(Cu)(Mg)(Zr)
Cu2O	CEF (SLN)	(2)(1)	(Ag,Cu)(O)
Cu2SnTi	CEF (ST3)	(2)(1)(1)	(Cu)(Sn)(Ti)
Cu2Ti	CEF (SLN)	(0.666667) (0.333333)	(Co,Cu,Fe,Ni)(Ti)
Cu2TiZr	CEF (ST3)	(0.5)(0.25) (0.25)	(Cu)(Ti)(Zr)
Cu33Mn50Si17	CEF (ST3)	(0.33)(0.5) (0.17)	(Cu)(Mn)(Si)
Cu3Mg2Si	CEF (ST3)	(0.5)(0.3333) (0.1667)	(Cu)(Mg)(Si)
Cu3Ni27Sn10	CEF (ST3)	(0.075)(0.675) (0.26)	(Cu)(Ni)(Sn)
Cu3Si4Zr2	CEF (ST3)	(0.3334) (0.4444) (0.2222)	(Cu)(Si)(Zr)
Cu3Sn	CEF (SLN)	(3)(1)	(Cu,Sn)(Cu,Sn)
Cu3Ti2	CEF (SLN)	(0.6)(0.4)	(Cu,Fe,Ni)(Co,Ti)
Cu41Sn11	CEF (SLN)	(41)(11)	(Cu,Sn)(Cu,Sn)
Cu4MgSn	CEF (ST3)	(0.666)(0.167)	(Cu)(Mg)(Sn)

Name	Model	Lattice Size	Constituent
		(0.167)	
Cu4MnSn	CEF (ST3)	(0.666)(0.167) (0.167)	(Cu)(Mn)(Sn)
Cu4Si2Zr3	CEF (ST3)	(0.4444) (0.2222) (0.3334)	(Cu)(Si)(Zr)
Cu4Si4Zr3	CEF (ST3)	(0.3636) (0.3636) (0.2728)	(Cu)(Si)(Zr)
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)
Cu55Mg22Si23	CEF (ST3)	(0.55)(0.22) (0.23)	(Cu)(Mg)(Si)
Cu6Sn5L	CEF (SLN)	(1)(1)(1)	(Cu)(Cu,Sn,Va)(Sn)
CuMg2	CEF (SLN)	(0.33333) (0.66667)	(Cu,Ni)(Mg)
CuMgSn	CEF (ST3)	(0.334)(0.333) (0.333)	(Cu)(Mg)(Sn)
CuMnZn	CEF (ST3)	(1)(1)(1)	(Cu)(Mn)(Zn)
CuNiTi_T1	CEF (SLN)	(0.6667) (0.3333)	(Cu,Ni)(Ti)
CuNiTi_T2	CEF (ST3)	(0.035)(0.565) (0.4)	(Cu)(Ni)(Ti)
CuNiTi_T3	CEF (ST3)	(0.035)(0.565) (0.4)	(Cu)(Ni)(Ti)
CuNiTi_T4	CEF (ST3)	(0.075)(0.675)	(Cu)(Ni)(Ti)

Name	Model	Lattice Size	Constituent
		(0.25)	
CuNiTi_T5	CEF (ST3)	(0.25)(0.5) (0.25)	(Cu)(Ni)(Ti)
CuNiTi_T6	CEF (ST3)	(0.25)(0.5) (0.25)	(Cu)(Ni)(Ti)
CuO	CEF (ST2)	(1)(1)	(Cu)(O)
CuSi12Zr12	CEF (ST3)	(0.04)(0.48) (0.48)	(Cu)(Si)(Zr)
CuSi2Zr	CEF (ST3)	(0.25)(0.5) (0.25)	(Cu)(Si)(Zr)
CuSi4Zr2	CEF (ST3)	(0.143)(0.571) (0.286)	(Cu)(Si)(Zr)
CuSiZr	CEF (ST3)	(0.3333) (0.3333) (0.3334)	(Cu)(Si)(Zr)
CuSn3Ti5	CEF (ST3)	(5)(3)(1)	(Ti)(Sn)(Cu)
CuSnTi	CEF (ST3)	(1)(1)(1)	(Cu)(Sn)(Ti)
CuSn_Gamma	CEF (SLN)	(1)	(Ag,Cu,Mg,Mn,Ni,Sn)
CuTi	CEF (SLN)	(0.5)(0.5)	(Co,Cu,Ni,Ti)(Cu,Ni,Ti,Zr)
CuZn_Beta	CEF (SLN)	(1)	(Cu,Zn)
CuZr	CEF (SLN)	(1)(1)	(Ag,Cu,Ni)(Ti,Zr)
D0_19	CEF (SLN)	(0.75)(0.25) (0.5)	(Al,Cr,Cu,Mn,Mo,Ni,Sn,Ti,V,Zr) (Al,Cr,Mn,Mo,Ni,Si,Sn,Ti)(C,Va)
D0_22	CEF (SLN)	(3)(1)	(Al,Mo,Si,Ti)(Al,Cr,Mo,Ti,Zr)
D0_22_TiAl3_L	CEF (SLN)	(3)(1)	(Al,Ti)(Al,Cr,Ti,V)
Delta_AlFeSi	CEF (SLN)	(5)(1)	(Al,Si)(Fe)

Name	Model	Lattice Size	Constituent
Delta_Cu33Si7	CEF (SLN)	(0.825)(0.175)	(Ag,Cu,Mg)(Si)
Diamond	CEF (SLN)	(1)	(Ag,Al,B,C,Ni,Si,Sn)
Eps	CEF (SLN)	(1)	(Al,Cu,Zn)
Epsilon_Cu15Si4	CEF (SLN)	(0.789474) (0.210526)	(Ag,Cu,Mg,Zn)(Al,Si)
Eta_Cu19Si6	CEF (SLN)	(0.76)(0.24)	(Ag,Cu,Mg)(Si)
Eta_MC	CEF (SLN)	(1)(1)	(Mo)(C,Va)
Fcc	CEF (SLN)	(1)(1)	(Ag,Al,Co,Cr,Cu,Fe,Hf,Li,Mg,Mn,Mo, Ni,Si,Sn,Ti,V,Zn,Zr)(B,C,O,Va)
Fcc_MC	CEF (SLN)	(1)(1)	(Co,Cr,Fe,Mo,Ni,Si,Ti,Zr)(C,Va)
Fe18Sn9Zr5	CEF (ST3)	(18)(9)(5)	(Fe)(Sn)(Zr)
Fe2Hf_C14	CEF (SLN)	(0.6667) (0.3333)	(Fe)(Fe,Hf)
Fe2Hf_C15	CEF (ST2)	(0.6667) (0.3333)	(Fe)(Hf)
Fe2Hf_C36	CEF (ST2)	(0.6667) (0.3333)	(Fe)(Hf)
Fe2Si	CEF (ST2)	(0.666667) (0.333333)	(Fe)(Si)
Fe2TiZn22	CEF (ST3)	(2)(1)(22)	(Fe)(Ti)(Zn)
Fe2V2Si	CEF (ST3)	(2)(2)(1)	(Fe)(V)(Si)
Fe3Sn2	CEF (ST2)	(3)(2)	(Fe)(Sn)
Fe3Sn9Zr20	CEF (ST3)	(3)(9)(20)	(Fe)(Sn)(Zr)
Fe4Sn10Zr9	CEF (ST3)	(4)(10)(9)	(Fe)(Sn)(Zr)
Fe4Sn4Zr3	CEF (ST3)	(4)(4)(3)	(Fe)(Sn)(Zr)
Fe4V5Si4	CEF (ST3)	(4)(5)(4)	(Fe)(V)(Si)

Name	Model	Lattice Size	Constituent
Fe5Ni3Si2	CEF (SLN)	(0.8)(0.2)	(Fe,Ni)(Si)
Fe5Sn3	CEF (ST2)	(5)(3)	(Fe)(Sn)
Fe5V3Si2	CEF (ST3)	(5)(3)(2)	(Fe)(V)(Si)
Fe6Sn6Zr	CEF (ST3)	(6)(6)(1)	(Fe)(Sn)(Zr)
Fe9Sn20Zr22	CEF (ST3)	(9)(20)(22)	(Fe)(Sn)(Zr)
FeHf2	CEF (ST2)	(0.3333) (0.6667)	(Fe)(Hf)
FeMn2Zn7	CEF (ST3)	(0.1)(0.2)(0.7)	(Fe)(Mn)(Zn)
FeMo4Zr9	CEF (ST3)	(1)(4)(9)	(Fe)(Mo)(Zr)
FeSi2_H	CEF (SLN)	(0.3)(0.7)	(Fe,V,Zr)(Al,Si)
FeSi2_L	CEF (SLN)	(1)(2)	(Co,Fe,Ni,V)(Al,Si)
FeSiZr_T1	CEF (ST3)	(1)(1)(1)	(Fe)(Si)(Zr)
FeSiZr_T3	CEF (ST3)	(4)(7)(4)	(Fe)(Si)(Zr)
FeSiZr_T4	CEF (ST3)	(41)(41)(18)	(Fe)(Si)(Zr)
FeSiZr_T5	CEF (SLN)	(16)(7)(6)	(Fe)(Fe,Si)(Zr)
FeSiZr_T8	CEF (ST3)	(4)(2)(1)	(Fe)(Si)(Zr)
FeSiZr_T9	CEF (ST3)	(29)(29)(42)	(Fe)(Zr)(Si)
FeSn	CEF (ST2)	(1)(1)	(Fe)(Sn)
FeSn2	CEF (ST2)	(1)(2)	(Fe)(Sn)
FeSn2Zr6	CEF (ST3)	(1)(2)(6)	(Fe)(Sn)(Zr)
FeZn_Delta	CEF (SLN)	(0.058)(0.18) (0.525)(0.237)	(Fe)(Al,Fe,Mn,Si,Zn)(Zn)(Zn)
FeZn_Gamma	CEF (SLN)	(0.154)(0.154) (0.231)(0.461)	(Fe,Mn,Zn)(Fe,Mn,Zn) (Al,Fe,Mn,Si,Zn)(Zn)
FeZn_Gamma1	CEF (SLN)	(0.137)(0.118) (0.745)	(Fe)(Al,Fe,Mn,Si,Zn)(Mn,Zn)

Name	Model	Lattice Size	Constituent
FeZn_Zeta	CEF (SLN)	(0.072)(0.856)(0.072)	(Fe,Mn,Va)(Al,Zn)(Al,Si,Zn,Va)
FeZr3	CEF (SLN)	(1)(3)	(Al,Fe,Zr)(Fe,Ti,Zr)
Gamma2	CEF (SLN)	(0.255)(0.745)	(Al,Fe,Mn,Zn)(Zn)
Gamma_AlFeSi	CEF (ST3)	(0.635)(0.205)(0.16)	(Al)(Fe)(Si)
Gamma_Cu56Si11	CEF (SLN)	(0.835821)(0.164179)	(Ag,Cu,Mg,Mn,Zn)(Si)
Gamma_H	CEF (SLN)	(4)(1)(8)	(Al,Si,Zn)(Al,Cu,Zn)(Cu,Fe,Mn)
Gammabrass	CEF (SLN)	(1)	(Al,Cu,Mn,Si,Zn)
Gas	GAS	(1)	(Ag,Al,AlO,AlO2,Al2,Al2O,Al2O2,Al2O3,C1O1,C1O2,Fe,FeO,FeO2,Fe2,Hf,HfO,HfO2,Li,Li2,Li2O,Li2O2,Mg,Mg2,MgO,Mn,O,O2,O3,Sn,Sn2,SnO,SnO2,Si,Si2,Si3,SiO,SiO2,Ti,TiO,TiO2,Zn,Zr,Zr2,ZrO,ZrO2)
Graphite	CEF (SLN)	(1)	(B,C)
H_CoMnSi	CEF (ST3)	(0.5)(0.25)(0.25)	(Co)(Mn)(Si)
H_L21	CEF (SLN)	(0.5)(0.5)(1)	(Al,Cr,Fe,Mn,Ni,Ti)(Al,Cr,Fe,Mn,Ni,Ti)(Cr,Fe,Mn,Ni,Va)
Halite	CEF (SLN)	(1)(1)	(Al+3,Co+2,Cr+3,Fe+2,Fe+3,Mg+2,Mn+2,Mn+3,Ni+2,V,V+2,V+3,Va)(O-2,Va)
Hcp	CEF (SLN)	(1)(0.5)	(Ag,Al,Co,Cr,Cu,Fe,Hf,Li,Mg,Mn,Mo,Ni,Si,Sn,Ti,V,Zn,Zr)(B,C,O,Va)
Hcp_M2C	CEF (SLN)	(1)(0.5)	(Co,Cr,Fe,Mo,Ni,Ti)(C,Va)

Name	Model	Lattice Size	Constituent
Hf3Si	CEF (ST2)	(0.75)(0.25)	(Hf)(Si)
Hf3Si2	CEF (ST2)	(2)(3)	(Si)(Hf)
Hf5Si3	CEF (ST2)	(3)(5)	(Si)(Hf)
Hf5Sn3	CEF (ST2)	(5)(3)	(Hf)(Sn)
Hf5Sn4	CEF (ST2)	(5)(4)	(Hf)(Sn)
HfMn	CEF (ST2)	(0.5)(0.5)	(Hf)(Mn)
HfMn2	CEF (SLN)	(1)(2)	(Hf,Mn)(Hf,Mn)
HfNiTi_Tao	CEF (SLN)	(11)(14)	(Ni)(Hf,Ti)
HfSi	CEF (ST2)	(0.5)(0.5)	(Hf)(Si)
HfSi2	CEF (SLN)	(1)(2)	(Hf,Si)(Si)
HfSiO4	CEF (ST3)	(1)(1)(4)	(Hf)(Si)(O)
HfSn2	CEF (ST2)	(1)(2)	(Hf)(Sn)
J_Co45Si40V15	CEF (ST3)	(0.45)(0.4) (0.15)	(Co)(Si)(V)
Ksi_Carbide	CEF (SLN)	(3)(1)	(Cr,Fe,Mo)(C)
L10_TiAl	CEF (SLN)	(1)(1)(2)	(Al,Cr,Mn,Mo,Ti,V,Zr) (Al,Cr,Mn,Mo,Ti,V,Zr)(C,Va)
L12_FCC	CEF (SLN)	(0.75)(0.25)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Ni,Si,Ti,V,Zr) (Al,Co,Cr,Cu,Fe,Mn,Mo,Ni,Si,Ti,V,Zr)
L12_Ti25Mn9Al66	CEF (ST3)	(0.67)(0.08) (0.25)	(Al)(Mn)(Ti)
L_CoMnSi	CEF (ST3)	(0.4433) (0.3333) (0.2233)	(Co)(Mn)(Si)
L_Sigma	CEF (SLN)	(8)(4)(18)	(Mn,Ni)(Cr)(Cr,Mn)
Laves_C14	CEF (SLN)	(2)(1)	(Al,Co,Cr,Cu,Fe,Hf,Li,Mg,Mn,Mo,Ni,

Name	Model	Lattice Size	Constituent
			Si,Ti,V,Zn,Zr)(Al,Co,Cr,Cu,Fe,Hf,Mg,Mn,Mo,Ni,Si,Ti,V,Zn,Zr)
Laves_C15	CEF (SLN)	(2)(1)	(Al,Co,Cr,Cu,Fe,Hf,Li,Mg,Mn,Mo,Ni,Si,Sn,Ti,V,Zn,Zr)(Al,Co,Cr,Cu,Fe,Hf,Li,Mg,Mn,Mo,Ni,Si,Sn,Ti,V,Zn,Zr)
Laves_C36	CEF (SLN)	(2)(1)	(Al,Co,Cr,Cu,Fe,Mg,Mn,Mo,Ni,Si,Ti,V,Zn,Zr)(Al,Co,Cr,Cu,Fe,Mg,Mn,Ni,Si,Sn,Ti,V,Zn,Zr)
Li12Mg3Si4	CEF (ST3)	(0.631579) (0.157895) (0.210526)	(Li)(Mg)(Si)
Li12Si7	CEF (ST2)	(0.6316) (0.3654)	(Li)(Si)
Li13Si4	CEF (ST2)	(0.7647) (0.2353)	(Li)(Si)
Li13Sn5	CEF (ST2)	(13)(5)	(Li)(Sn)
Li17Si4	CEF (ST2)	(0.8095) (0.1905)	(Li)(Si)
Li21Si5	CEF (ST2)	(0.80769) (0.19231)	(Li)(Si)
Li22Sn5	CEF (ST2)	(22)(5)	(Li)(Sn)
Li2C2_T1	CEF (ST2)	(0.5)(0.5)	(C)(Li)
Li2C2_T2	CEF (ST2)	(0.5)(0.5)	(C)(Li)
Li2MgSi	CEF (ST3)	(0.5)(0.25) (0.25)	(Li)(Mg)(Si)
Li2O2	CEF (ST2)	(2)(1)	(Li+1)(O2-2)
Li2Sn5	CEF (ST2)	(2)(5)	(Li)(Sn)

Name	Model	Lattice Size	Constituent
Li4.13Si	CEF (ST2)	(0.80488) (0.19512)	(Li)(Si)
Li5Sn2	CEF (ST2)	(5)(2)	(Li)(Sn)
Li7Si3	CEF (ST2)	(0.7)(0.3)	(Li)(Si)
Li7Sn2	CEF (ST2)	(7)(2)	(Li)(Sn)
Li7Sn3	CEF (ST2)	(7)(3)	(Li)(Sn)
Li8MgSi6	CEF (ST3)	(0.533333) (0.066667) (0.4)	(Li)(Mg)(Si)
LiC6	CEF (ST2)	(6)(1)	(C)(Li)
LiSi	CEF (ST2)	(0.5)(0.5)	(Li)(Si)
LiSn	CEF (ST2)	(1)(1)	(Li)(Sn)
LiZn2	CEF (ST2)	(1)(2)	(Li)(Zn)
Liquid	CEF (SLN)	(1)	(Ag,Al,B,C,Co,Cr,Cu,Fe,Hf,Li,Mg, Mg2Sn,Mn,Mo,Ni,Si,Sn,Ti,V,Zn,Zr, Al2O3,B2O3,CoO,Co2O3,Cr2/3O, CuO,Cu2O,Cu2O3,FeO,FeO3/2, HfO2,Li2O,MgO,MnO,MnO3/2,MoO2, MoO3,NiO,O,SiO2,SnO,SnO2,TiO, TiO3/2,TiO2,VO,VO2,VO3/2, VO5/2,Zr1/2O)
M10X7_oS68	CEF (SLN)	(10)(7)	(Ag,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,Ni,V)(C)

Name	Model	Lattice Size	Constituent
M23X6_cF116	CEF (SLN)	(23)(6)	(Co,Cu,Fe,Si)(Hf,Zr)
M2B_tI12	CEF (SLN)	(2)(1)	(Co,Fe,Mn,Mo,Ni)(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)
M2X_tI12	CEF (SLN)	(0.333)(0.667)	(Al,Si)(Cr,Fe,Hf,Mn,Mo,Ti,V,Zr)
M3C2	CEF (SLN)	(3)(2)	(Co,Cr,Mo,V)(C)
M51X14_hP68	CEF (SLN)	(51)(14)	(Ag,Cu,Ni)(Hf,Ti,Zr)
M5C2	CEF (SLN)	(5)(2)	(Fe,Mn,V)(C)
M5Si3_tI32	CEF (SLN)	(0.625)(0.375)	(Cr,Fe,Mo,Si,Ti,V,Zr)(Al,Mo,Ni,Si)
M5Si4_tP36	CEF (SLN)	(0.555556) (0.444444)	(Cr,Hf,Mo,Ti,Zr)(Al,Si)
M5X3_hP16	CEF (SLN)	(2)(3)(3)	(Al,Co,Cr,Cu,Fe,Mn,Mo,Ni,Si,Ti,V,Zr) (Al,Cr,Ni,Si,Sn,Ti) (Co,Cr,Cu,Fe,Mn,Mo,Ni,Ti,V)
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) (Co,Cr,Fe,Mo,Ni,Si,V)(C)
M6Sn5	CEF (SLN)	(1)(1)(1)	(Cu,Ni)(Cu,Sn,Ni,Va)(Sn)
M7C3	CEF (SLN)	(7)(3)	(Co,Cr,Fe,Mn,Mo,Ni,V)(C)
M7X2_mS36	CEF (SLN)	(7)(2)	(Al,Cr,Cu,Fe,Ni,V)(Cr,Hf,Ti,Zr)
M8X3_oP44	CEF (SLN)	(8)(3)	(Ag,Cu)(Hf,Zr)
MAl3Si3Zr5	CEF (SLN)	(3)(5)	(Al,Cu,Si)(Zr)
MB2_hP3	CEF (SLN)	(1)(2)	(Al,Cr,Hf,Mg,Mn,Mo,Ti,V,Zr,Va)(B,Va)
MB_oP8	CEF (SLN)	(1)(1)	(Co,Fe,Mn,Ti)(B)
MB_oS8	CEF (SLN)	(1)(1)	(Cr,Mo,Ni,V)(B,Va)
MO2_cF12	CEF (SLN)	(1)(2)	(Hf,Zr)(O,Va)

Name	Model	Lattice Size	Constituent
MO2_mP12	CEF (SLN)	(1)(2)	(Hf,Mo,V,Zr)(O)
MO2_tP6	CEF (SLN)	(1)(2)	(Hf,Zr)(O,Va)
MSi	CEF (SLN)	(0.5)(0.5)	(Co,Cr,Fe,Mg,Mn,Ni,Si,V,Zr) (Al,Co,Cr,Si)
MSi2	CEF (SLN)	(1)(2)	(Co,Fe,Mn,Ni,Zr)(Al,Si)
MX2_cF96	CEF (SLN)	(1)(2)	(Co,Cr,Cu,Fe,Hf,Ni,Si,Ti) (Al,Cu,Fe,Hf,Ni,Ti,V,Zr)
MX2_tI12	CEF (SLN)	(1)(2)	(Al,Co,Cu,Fe,Ni,Si,Zr)(Fe,Hf,Ti,Zr)
MX2_tI6	CEF (SLN)	(1)(2)	(Ag,Co,Cu,Fe,Ni)(Al,Hf,Ti,Zr)
MX_oS8	CEF (SLN)	(1)(1)	(Cu,Ni)(Hf,Ti,Zr)
Mg2C3	CEF (ST2)	(0.4)(0.6)	(Mg)(C)
Mg2CrNi	CEF (SLN)	(0.12)(0.33) (0.55)	(Cr,Ni)(Mg,Ni)(Cr,Mg)
Mg2M	CEF (SLN)	(0.5)(0.25) (0.25)	(Mg)(Al,Si,Sn)(Li,Va)
Mg2Ni	CEF (SLN)	(2)(1)	(Cr,Mg)(Cu,Ni,Zn)
Mg2SiNi3	CEF (ST3)	(2)(1)(3)	(Mg)(Si)(Ni)
Mg2Zn11	CEF (SLN)	(5)(6)(2)	(Al,Zn)(Cu,Zn)(Mg)
Mg2Zn3	CEF (SLN)	(2)(3)	(Mg)(Al,Zn)
Mg3MnNi2	CEF (ST3)	(3)(1)(2)	(Mg)(Mn)(Ni)
Mg3Ni11Si6	CEF (ST3)	(3)(11)(6)	(Mg)(Ni)(Si)
Mg5Ni17Si7	CEF (SLN)	(5)(17)(7)	(Mg)(Ni,Si)(Ni,Si)
Mg7Zn3	CEF (ST2)	(51)(20)	(Mg)(Zn)
MgB4	CEF (ST2)	(1)(4)	(Mg)(B)
MgB7	CEF (ST2)	(1)(7)	(Mg)(B)
MgC2	CEF (ST2)	(0.333333)	(Mg)(C)

Name	Model	Lattice Size	Constituent
		(0.666667)	
MgNi8Si6	CEF (ST3)	(1)(8)(5.5)	(Mg)(Ni)(Si)
MgZn	CEF (SLN)	(12)(13)	(Mg)(Al,Zn)
Mn11Si19	CEF (SLN)	(11)(19)	(Mn,Ni)(Al,Si)
Mn13NiSi6	CEF (ST3)	(13)(1)(6)	(Mn)(Ni)(Si)
Mn19Sn6	CEF (ST2)	(19)(6)	(Mn)(Sn)
Mn2Ni3Si	CEF (ST3)	(1)(1.56) (0.44)	(Mn)(Ni)(Si)
Mn2NiSi	CEF (SLN)	(2)(1)(1)	(Mn,Ni)(Mn,Ni)(Si)
Mn2Sn	CEF (ST2)	(2)(1)	(Mn)(Sn)
Mn3B4	CEF (ST2)	(0.428571) (0.571429)	(Mn)(B)
Mn3Ni10Si7	CEF (ST3)	(3)(10)(7)	(Mn)(Ni)(Si)
Mn3Ni2Si	CEF (ST3)	(3)(2)(1)	(Mn)(Ni)(Si)
Mn3Ni9Si8	CEF (ST3)	(3)(9)(8)	(Mn)(Ni)(Si)
Mn3Si	CEF (SLN)	(3)(1)	(Cr,Fe,Mn,Ni)(Al,Si)
Mn3Ti	CEF (SLN)	(3)(1)	(Mn,V)(Ti)
Mn4Ti	CEF (SLN)	(0.815)(0.185)	(Mn,V)(Ti)
Mn52Ni29Si19	CEF (ST3)	(52)(29)(19)	(Mn)(Ni)(Si)
Mn61Ni12Si27	CEF (ST3)	(61)(12)(27)	(Mn)(Ni)(Si)
Mn6Ni16Si7	CEF (ST3)	(6)(16)(7)	(Mn)(Ni)(Si)
Mn6Si	CEF (SLN)	(0.85)(0.15)	(Al,Mn)(Si)
Mn9Si2	CEF (ST2)	(0.825)(0.175)	(Mn)(Si)
MnB4	CEF (ST2)	(0.2)(0.8)	(Mn)(B)
MnNi2	CEF (SLN)	(1)(2)	(Mn,Ni)(Ni)

Name	Model	Lattice Size	Constituent
MnNiSi	CEF (ST3)	(1)(1)(1)	(Mn)(Ni)(Si)
MnNiSi_P	CEF (SLN)	(1)(1)(1)	(Mn)(Ni)(Ni,Si)
MnNi_Beta	CEF (SLN)	(1)(1)	(Co,Cr,Fe,Mg,Mn,Ni)(Co,Cr,Fe,Mn,Ni)
MnSi	CEF (ST2)	(1)(1)	(Mn)(Si)
MnSn2	CEF (ST2)	(1)(2)	(Mn)(Sn)
MnZn9	CEF (ST2)	(0.1)(0.9)	(Mn)(Zn)
Mo2B5	CEF (SLN)	(2)(5)	(Mo)(B,Va)
Mo2Hf	CEF (SLN)	(2)(1)	(Hf,Mo)(Hf,Mo)
Mo2Ti	CEF (ST2)	(2)(1)	(Mo)(Ti)
Mo3Si5Zr2	CEF (ST3)	(3)(5)(2)	(Mo)(Si)(Zr)
Mo3Sn	CEF (ST2)	(3)(1)	(Mo)(Sn)
Mo3Ti2	CEF (ST2)	(3)(2)	(Mo)(Ti)
Mo4O11	CEF (ST2)	(0.266667) (0.733333)	(Mo)(O)
Mo4Si9Ti7	CEF (SLN)	(0.55)(0.45)	(Mo,Ti)(Si)
Mo4Ti	CEF (ST2)	(4)(1)	(Mo)(Ti)
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)	(0.258064) (0.741935)	(Mo)(O)
Mo9O26	CEF (ST2)	(0.257143) (0.742857)	(Mo)(O)
Mo9Ti	CEF (ST2)	(9)(1)	(Mo)(Ti)
MoB4	CEF (ST2)	(0.8)(0.2)	(B)(Mo)
MoNi	CEF (SLN)	(24)(20)(12)	(Co,Cr,Fe,Ni)

Name	Model	Lattice Size	Constituent
			(Al,Co,Cr,Fe,Mn,Mo,Ni)(Mo)
MoNi3	CEF (SLN)	(0.75)(0.25)	(Mo,Ni)(Mo,Ni,Ti)
MoNi4	CEF (ST2)	(0.2)(0.8)	(Mo)(Ni)
MoO3	CEF (ST2)	(1)(3)	(Mo)(O)
MoSi2	CEF (SLN)	(1)(2)	(Co,Cr,Mo,V)(Al,Si)
MoSi6Ti2	CEF (SLN)	(1)(2)	(Mo,Ti)(Si)
MoSiZr	CEF (ST3)	(1)(1)(1)	(Mo)(Si)(Zr)
MoSn	CEF (ST2)	(1)(1)	(Mo)(Sn)
MoSn2	CEF (ST2)	(1)(2)	(Mo)(Sn)
MoTi	CEF (ST2)	(1)(2)	(Mo)(Ti)
MoTi2	CEF (ST2)	(1)(2)	(Mo)(Ti)
Mu_PHASE	CEF (SLN)	(7)(2)(4)	(Al,Co,Cr,Fe,Mo,Mn,Ni,Si,Ti,V,Zr) (Mo)(Al,Co,Cr,Fe,Mo,Ni,Si,Ti,V,Zr)
Ni11Si31Zr8	CEF (ST3)	(0.22)(0.62) (0.16)	(Ni)(Si)(Zr)
Ni11Si5Zr4	CEF (ST3)	(0.55)(0.25) (0.2)	(Ni)(Si)(Zr)
Ni16Si7Ti6	CEF (SLN)	(16)(7)(6)	(Ni)(Si)(Si,Ti)
Ni2Si2Zr	CEF (ST3)	(0.4)(0.4)(0.2)	(Ni)(Si)(Zr)
Ni2Si9Zr14	CEF (ST3)	(0.08)(0.36) (0.56)	(Ni)(Si)(Zr)
Ni2SiO4	CEF (ST3)	(2)(1)	(NiO)(SiO2)
Ni2SiZn	CEF (ST3)	(2)(1)(1)	(Ni)(Si)(Zn)
Ni2SiZn3	CEF (ST3)	(2)(1)(3)	(Ni)(Si)(Zn)
Ni2Si_H	CEF (SLN)	(1)(1)(1)	(Ni)(Ni,Va)(Al,Si)
Ni2Si_L	CEF (SLN)	(2)(1)	(Fe,Ni)(Al,Si)

Name	Model	Lattice Size	Constituent
Ni2SnTi	CEF (SLN)	(0.25)(0.5) (0.25)	(Ti)(Ni,Va)(Sn,Ti)
Ni2Ti2Sn	CEF (ST3)	(0.4)(0.4)(0.2)	(Ti)(Ni)(Sn)
Ni2V	CEF (SLN)	(0.6667) (0.3333)	(Ni)(Al,V)
Ni2Zr	CEF (SLN)	(0.04)(0.66) (0.3)	(Cu,Zr)(Ni)(Zr)
Ni3B	CEF (ST2)	(3)(1)	(Ni)(B)
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)
Ni3Si2Zn	CEF (ST3)	(3)(2)(1)	(Ni)(Si)(Zn)
Ni3SiTi2	CEF (SLN)	(3)(1)(2)	(Ni,Si)(Ni,Si)(Ti)
Ni3Si_H	CEF (SLN)	(3)(1)	(Ni)(Al,Si)
Ni3Si_L	CEF (SLN)	(3)(1)	(Ni)(Si,Ti)
Ni3Sn2	CEF (SLN)	(0.5)(0.25) (0.25)	(Ni,Sn)(Ni)(Ni)
Ni3Sn4	CEF (SLN)	(0.4286) (0.5714)	(Cu,Ni)(Ni,Sn)
Ni3Ti	CEF (SLN)	(0.75)(0.25)	(Co,Cr,Cu,Fe,Ni,Ti) (Cr,Cu,Fe,Hf,Mo,Ni,Si,Ti,V)
Ni3V	CEF (SLN)	(3)(1)	(Fe,Ni,V)(Al,Ni,Ti,V)
Ni3Zr	CEF (ST2)	(3)(1)	(Ni)(Zr)
Ni4Si3Ti	CEF (SLN)	(4)(3)(1)	(Ni,Ti)(Si)(Ti)
Ni4Si7Ti4	CEF (SLN)	(4)(7)(4)	(Ni)(Si,Ti)(Si,Ti)
Ni4Si9Zr7	CEF (ST3)	(0.2)(0.45)	(Ni)(Si)(Zr)

Name	Model	Lattice Size	Constituent
		(0.35)	
Ni5Si2	CEF (SLN)	(5)(2)	(Fe,Ni)(Al,Si)
Ni5SiTi6	CEF (ST3)	(5)(1)(6)	(Ni)(Si)(Ti)
Ni7Hf3	CEF (ST2)	(7)(3)	(Ni)(Hf)
Ni9Si2Zn	CEF (ST3)	(9)(2)(1)	(Ni)(Si)(Zn)
NiSi	CEF (SLN)	(1)(1)	(Fe,Ni,Zn)(Si)
NiSi4Ti4	CEF (ST3)	(1)(4)(4)	(Ni)(Si)(Ti)
NiSiTi	CEF (SLN)	(1)(1)(1)	(Ni,Ti)(Si)(Ni,Ti)
NiSiZr	CEF (ST3)	(0.3333) (0.3333) (0.3334)	(Ni)(Si)(Zr)
NiSnTi	CEF (ST3)	(0.333)(0.333) (0.333)	(Ti)(Ni)(Sn)
NiTiZr	CEF (SLN)	(1)(1)(1)	(Ni,Ti,Zr)(Ni,Ti,Zr)(Ni,Ti,Zr)
NiV3	CEF (ST2)	(0.25)(0.75)	(Ni)(V)
NiZn8	CEF (ST2)	(0.111)(0.889)	(Ni)(Zn)
NiZn_Beta1	CEF (SLN)	(1)(1)	(Al,Cu,Ni,Zn)(Ni,Zn)
NiZn_Gamma	CEF (SLN)	(1)	(Ni,Zn)
P_Phase	CEF (SLN)	(24)(12)(20)	(Co,Cr,Fe,Ni)(Mo)(Co,Cr,Fe,Mo,Ni)
Phi_Al2Mg5Zn2	CEF (SLN)	(6)(5)	(Mg)(Al,Zn)
Q	CEF (ST3)	(0.4375) (0.375) (0.1875)	(Al)(Mg)(Cu)
Q_Al5Cu2Mg8Si6	CEF (ST4)	(0.2381) (0.0952) (0.381)	(Al)(Cu)(Mg)(Si)

Name	Model	Lattice Size	Constituent
		(0.2857)	
Quartz	CEF (ST2)	(1)(2)	(Si)(O)
R_Al5CuLi3	CEF (ST3)	(0.55)(0.117) (0.333)	(Al)(Cu)(Li)
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,Mo,Mn,Ni,V)(Cr,Mo) (Co,Cr,Fe,Mn,Mo,Ni,Si,V)
Rutile	CEF (SLN)	(1)(2)	(Mn+4,Sn+4,Ti+3,Ti+4,V+4)(O-2,Va)
S	CEF (ST3)	(0.5)(0.25) (0.25)	(Al)(Mg)(Cu)
Shp_MC	CEF (ST2)	(1)(1)	(Mo)(C)
Si2Ti	CEF (SLN)	(0.666667) (0.333333)	(Al,Si)(Co,Cr,Mo,Ti,V)
Si2TiV	CEF (SLN)	(1)(1)	(Si)(Ti,V)
Si2V	CEF (SLN)	(0.666667) (0.333333)	(Al,Si)(Fe,Mo,Ti,V)
Si2Zr	CEF (SLN)	(2)(1)	(Si,Al)(Al,Co,Fe,Zr)
Si2Zr3	CEF (SLN)	(2)(3)	(Co,Si)(Zr)
Si3Zr5	CEF (SLN)	(3)(5)	(Al,Mo,Si)(Zr)
Si4Ti5	CEF (SLN)	(0.444444) (0.555556)	(Si)(Mo,Ti)
Si4Zr5	CEF (SLN)	(4)(5)	(Al,Co,Si)(Zr)
Si5V6	CEF (SLN)	(0.454545) (0.545455)	(Si)(Cr,V)

Name	Model	Lattice Size	Constituent
SiB3	CEF (SLN)	(6)(2)(6)	(B)(Si)(B,Si)
SiB6	CEF (SLN)	(210)(23)(48)	(B)(Si)(B,Si)
SiBn	CEF (SLN)	(61)(1)(8)	(B)(Si)(B,Si)
SiC	CEF (ST2)	(1)(1)	(C)(Si)
SiTi	CEF (SLN)	(0.5)(0.5)	(Al,Si)(Co,Ti)
SiTi3	CEF (SLN)	(0.25)(0.75)	(Si)(Ti,V)
SiZr	CEF (SLN)	(1)(1)	(Si,Al)(Zr)
SiZr3	CEF (ST2)	(1)(3)	(Si)(Zr)
Sigma	CEF (SLN)	(8)(4)(18)	(Al,Co,Cr,Cu,Fe,Mn,Ni,Si) (Cr,Fe,Hf,Mo,Si,Ti,V) (Al,Co,Cr,Fe,Hf,Mn,Mo,Ni,Si,Ti,V)
Sn2V	CEF (ST2)	(1)(2)	(V)(Sn)
Sn2Zr	CEF (ST2)	(2)(1)	(Sn)(Zr)
Sn3Ti2	CEF (ST2)	(0.6)(0.4)	(Sn)(Ti)
Sn3Zr5_hP18	CEF (SLN)	(5)(3)(1)	(Ti,Zr)(Sn)(Sn,Va)
Sn5Ti6	CEF (SLN)	(0.455)(0.545)	(Sn)(Cr,Cu,Ni,Ti)
SnTi2	CEF (SLN)	(0.333)(0.667)	(Sn)(Co,Cr,Ti,Zr)
SnV3	CEF (SLN)	(0.25)(0.75)	(Sn,V)(V)
SnZr4	CEF (SLN)	(3)(1)	(Sn,Zr)(Sn,Zr)
Spinel	CEF (SLN)	(1)(2)(2)(4)	(Al+3,Co+2,Cr+2,Cr+3,Fe+2,Fe+3, Mg+2,Mn+2,Ni+2) (Al+3,Co+3,Cr+3, Fe+2,Fe+3,Mg+2,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)

Name	Model	Lattice Size	Constituent
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_Al2CuLi	CEF (ST3)	(0.5)(0.25) (0.25)	(Al)(Cu)(Li)
T1_AlCuMo	CEF (ST3)	(2.5)(0.5)(1)	(Al)(Cu)(Mo)
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)
T1_CoMnSi	CEF (ST3)	(0.08)(0.64) (0.28)	(Co)(Mn)(Si)
T1_CuFeTi	CEF (SLN)	(0.63)(0.37)	(Cu,Fe)(Ti)
T2_Al6CuLi3	CEF (ST3)	(0.57)(0.11) (0.32)	(Al)(Cu)(Li)
T2_AlCuMo	CEF (ST3)	(7.7)(2.3)(1)	(Al)(Cu)(Mo)
T2_CoMnSi	CEF (ST3)	(0.2456) (0.5088) (0.2456)	(Co)(Mn)(Si)
T2_CuFeTi	CEF (SLN)	(0.55)(0.45)	(Cu,Fe)(Ti)
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)	(Al,Si)(Fe)

Name	Model	Lattice Size	Constituent
		(0.33333)	
TAl3Zr	CEF (ST3)	(0.65)(0.1) (0.25)	(Al)(Si)(Zr)
T_AlCoMo	CEF (ST3)	(2.72)(0.28) (1)	(Al)(Co)(Mo)
T_AlCuMg	CEF (SLN)	(26)(6)(48)(1)	(Mg)(Al,Mg)(Al,Cu,Mg)(Al)
T_AlMgZn	CEF (SLN)	(26)(6)(48)(1)	(Mg)(Al,Mg)(Al,Cu,Mg,Zn)(Al)
T_Cu5Li2Mg11	CEF (ST3)	(0.278)(0.111) (0.611)	(Cu)(Li)(Mg)
T_FeNiZn	CEF (SLN)	(1)(5)	(Fe,Ni,Zn)(Zn)
Tau10_AlCuZr	CEF (ST3)	(0.241)(0.552) (0.207)	(Al)(Cu)(Zr)
Tau1_AlCrSi	CEF (ST3)	(13)(4)(4)	(Al)(Cr)(Si)
Tau1_AlCuZr	CEF (ST3)	(0.14)(0.71) (0.15)	(Al)(Cu)(Zr)
Tau1_AlFeZr	CEF (SLN)	(12)(1)	(Al,Fe)(Zr)
Tau1_AlNiZr	CEF (ST3)	(1)(1)(1)	(Al)(Ni)(Zr)
Tau1_AlSiZr	CEF (ST3)	(0.35)(0.39) (0.26)	(Al)(Si)(Zr)
Tau1_CoSiZr	CEF (ST3)	(1)(1)(1)	(Co)(Si)(Zr)
Tau1_NiSiV	CEF (SLN)	(1)(1)(1)	(Ni,Si)(Si)(V)
Tau2_AlCrSi	CEF (ST3)	(9)(3)(1)	(Al)(Cr)(Si)
Tau2_AlCuZr	CEF (ST3)	(0.13)(0.14) (0.73)	(Al)(Cu)(Zr)
Tau2_AlFeZr	CEF (SLN)	(1)(2)(6)	(Fe)(Al,Zr)(Zr)
Tau2_AlNiZr	CEF (ST3)	(1)(2)(1)	(Al)(Ni)(Zr)

Name	Model	Lattice Size	Constituent
Tau2_AlSiZr	CEF (ST3)	(0.65)(0.1)(0.25)	(Al)(Si)(Zr)
Tau2_Co5Si3Zr	CEF (ST3)	(5)(3)(1)	(Co)(Si)(Zr)
Tau2_NiSiV	CEF (SLN)	(2)(1)(3)	(Ni)(Ni,Si)(Ni,V)
Tau3_AlCrSi	CEF (SLN)	(11)(4)	(Al,Si)(Cr)
Tau3_AlCuZr	CEF (ST3)	(0.21)(0.28)(0.51)	(Al)(Cu)(Zr)
Tau3_AlFeZr	CEF (ST3)	(7)(67)(26)	(Fe)(Al)(Zr)
Tau3_AlNiZr	CEF (ST3)	(1)(4)(5)	(Al)(Ni)(Zr)
Tau3_CoSi2Zr	CEF (ST3)	(1)(2)(1)	(Co)(Si)(Zr)
Tau3_NiSiV	CEF (ST3)	(12)(5)(3)	(Ni)(Si)(V)
Tau4_AlCrSi	CEF (ST3)	(0.58)(0.315)(0.105)	(Al)(Cr)(Si)
Tau4_AlCuZr	CEF (ST3)	(0.25)(0.5)(0.25)	(Al)(Cu)(Zr)
Tau4_AlNiZr	CEF (ST3)	(2)(1)(6)	(Al)(Ni)(Zr)
Tau4_CoSi2Zr2	CEF (ST3)	(1)(2)(2)	(Co)(Si)(Zr)
Tau4_NiSiV	CEF (SLN)	(11)(3)(6)	(Ni)(Si)(Ni,V)
Tau5_AlNiZr	CEF (SLN)	(15)(8)(6)	(Al)(Al,Ni)(Zr)
Tau5_Co2Si2Zr	CEF (ST3)	(2)(2)(1)	(Co)(Si)(Zr)
Tau5_NiSiV	CEF (ST3)	(5)(3)(4)	(Ni)(Si)(V)
Tau6_AlCuZr	CEF (ST3)	(0.375)(0.5)(0.125)	(Al)(Cu)(Zr)
Tau6_AlNiZr	CEF (ST3)	(5)(2)(1)	(Al)(Ni)(Zr)
Tau6_Co7Si9Zr4	CEF (ST3)	(7)(9)(4)	(Co)(Si)(Zr)
Tau6_NiSiV	CEF (ST3)	(36)(23)(41)	(Ni)(Si)(V)

Name	Model	Lattice Size	Constituent
Tau7_AlCuZr	CEF (SLN)	(0.5)(0.423)(0.077)	(Al,Cu)(Cu)(Zr)
Tau7_CoSi10Zr9	CEF (ST3)	(1)(10)(9)	(Co)(Si)(Zr)
Tau8_AlCuZr	CEF (ST3)	(0.625)(0.125)(0.25)	(Al)(Cu)(Zr)
Tau9_AlCuZr	CEF (ST3)	(0.672)(0.157)(0.171)	(Al)(Cu)(Zr)
Tau_AlSiV	CEF (ST3)	(0.6)(1.4)(1)	(Al)(Si)(V)
Tb_Al7Cu4Li	CEF (ST3)	(0.6)(0.32)(0.08)	(Al)(Cu)(Li)
Ti10O19	CEF (ST2)	(10)(19)	(Ti)(O)
Ti20O39	CEF (ST2)	(20)(39)	(Ti)(O)
Ti2Zn	CEF (ST2)	(2)(1)	(Ti)(Zn)
Ti3B4	CEF (ST2)	(3)(4)	(Ti)(B)
Ti3O2	CEF (ST2)	(3)(2)	(Ti)(O)
Ti3O5	CEF (ST2)	(3)(5)	(Ti)(O)
Ti3Zn22	CEF (ST2)	(3)(22)	(Ti)(Zn)
Ti4O7	CEF (ST2)	(4)(7)	(Ti)(O)
Ti5O9	CEF (ST2)	(5)(9)	(Ti)(O)
Ti6O11	CEF (ST2)	(6)(11)	(Ti)(O)
Ti7O13	CEF (ST2)	(7)(13)	(Ti)(O)
Ti8O15	CEF (ST2)	(8)(15)	(Ti)(O)
Ti9O17	CEF (ST2)	(9)(17)	(Ti)(O)
TiAlSi_Tau1	CEF (SLN)	(8)(16)	(Al,Ti)(Al,Si)
TiAlSi_Tau2	CEF (SLN)	(1)(2)	(Ti)(Al,Si)
TiOx	CEF (SLN)	(1)(1)(1)	(Ti+2,Ti+3,Va)(Ti,Va)(O-2)

Name	Model	Lattice Size	Constituent
TiZn	CEF (ST2)	(1)(1)	(Ti)(Zn)
TiZn16	CEF (ST2)	(1)(16)	(Ti)(Zn)
TiZn2	CEF (ST2)	(1)(2)	(Ti)(Zn)
TiZn3	CEF (ST2)	(1)(3)	(Ti)(Zn)
Tridymite	CEF (ST2)	(1)(2)	(Si)(O)
V	CEF (ST3)	(0.38461) (0.15385) (0.46154)	(Al)(Mg)(Cu)
V2B3	CEF (ST2)	(2)(3)	(V)(B)
V2O5	CEF (ST2)	(2)(5)	(V)(O)
V2O_SS	CEF (SLN)	(1)(0.5)	(V)(O,Va)
V3B2	CEF (ST2)	(3)(2)	(V)(B)
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)
V4Zn5	CEF (ST2)	(4)(5)	(V)(Zn)
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)

Name	Model	Lattice Size	Constituent
VZn16	CEF (ST2)	(1)(16)	(V)(Zn)
VZn3	CEF (ST2)	(1)(3)	(V)(Zn)
W_CoMnSi	CEF (ST3)	(0.3333) (0.3333) (0.3333)	(Co)(Mn)(Si)
X_Co52Co20V28	CEF (ST3)	(0.52)(0.2) (0.28)	(Co)(Si)(V)
X_CoMnSi	CEF (ST3)	(0.4)(0.4459) (0.1541)	(Co)(Mn)(Si)
Zn22Zr	CEF (ST2)	(0.956522) (0.0434783)	(Zn)(Zr)
Zn2Zr	CEF (ST2)	(0.666667) (0.333333)	(Zn)(Zr)
Zn2Zr3	CEF (ST2)	(0.4)(0.6)	(Zn)(Zr)
Zn39Zr5	CEF (ST2)	(0.886364) (0.113636)	(Zn)(Zr)
Zn3Zr_h	CEF (ST2)	(0.75)(0.25)	(Zn)(Zr)
Zn3Zr_l	CEF (ST2)	(0.75)(0.25)	(Zn)(Zr)
ZnO	CEF (ST2)	(1)(1)	(Zn)(O)
ZnZr	CEF (ST2)	(0.5)(0.5)	(Zn)(Zr)
ZnZr2	CEF (ST2)	(0.333333) (0.666667)	(Zn)(Zr)
Zr2O	CEF (ST2)	(2)(1)	(Zr)(O)
Zr3O	CEF (ST2)	(3)(1)	(Zr)(O)
Zr6O	CEF (ST2)	(6)(1)	(Zr)(O)
ZrB	CEF (ST2)	(1)(1)	(Zr)(B)

Name	Model	Lattice Size	Constituent
ZrB12	CEF (ST2)	(1)(12)	(Zr)(B)
m_Ni4B3	CEF (ST2)	(0.564)(0.436)	(Ni)(B)
o_Ni4B3	CEF (ST2)	(0.586)(0.414)	(Ni)(B)