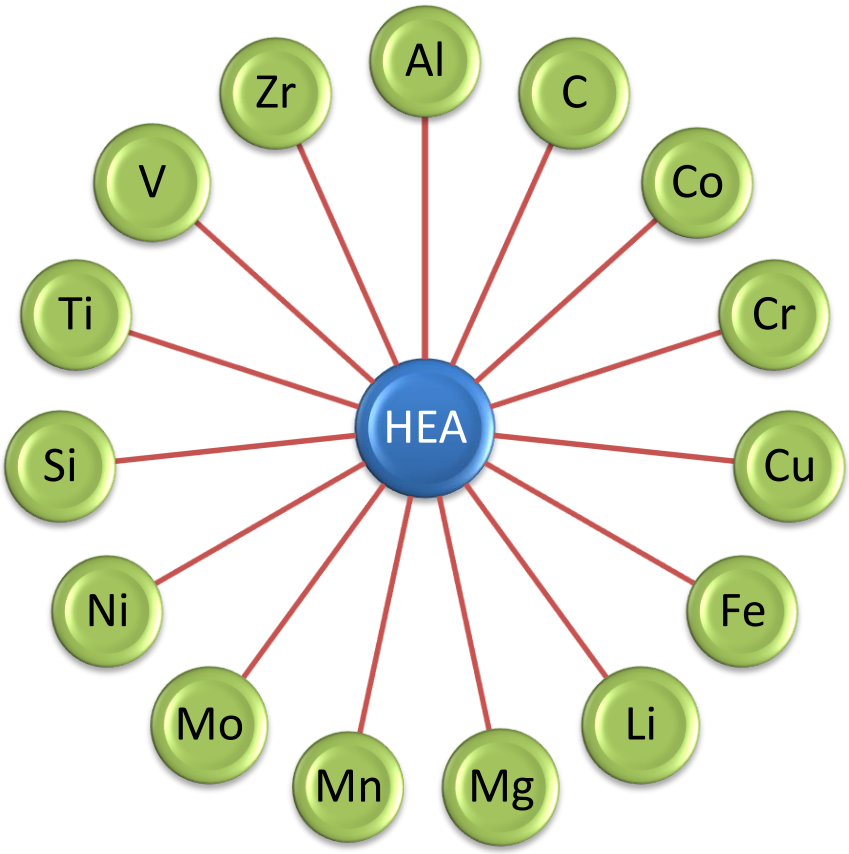
1. PanHEA

Thermodynamic database for multi-component high entropy alloys (HEA)



Copyright © CompuTherm LLC

1.1 Components

Total of 15 components are included in the database as listed here:

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

Minor alloying element: C

1.2 Suggested Composition Range

The suggested composition range for each element is listed in Table 1.1. 102/105 constituent binary systems have been modeled in the Al-C-Co-Cr-Cu-Fe-Li-Mg-Mn-Mo-Ni-Si-Ti-V-Zr fifteen-component system. There are 210/364 constituent ternaries have been modeled in the Al-Co-Cr-Cu-Fe-Li-Mg-Mn-Mo-Ni-Si-Ti-V-Zr fourteen-component system. The suggested composition ranges for these elements are given below:

Table 1.1: Suggested composition range

Element	Composition Range (at.%)
Al, Co, Cr, Cu, Fe, Li, Mg, Mn, Mo, Ni, Si, Ti, V, Zr	0 ~ 100
C	0~10

1.3 What's new in PanHEA2020

Major improvements of PanHEA2020 include (1) the addition of Mo and C into the database, (2) enhancement of the descriptions for the Laves_C14, Laves_C15, Laves_C36, and $L2_1$ phases. In addition, the modeling depth was extended in descriptions concerning mutual interactions of components in multicomponent alloys.

1.4 Phases

Total of 434 phases are included in the current database. The names and thermodynamic models of some phases are given in Table 1.2. Information on

all phases can be displayed in the TDB Viewer of Pandat or can be found at www.computherm.com.

Table 1.2: Phase name and related information

Name	Lattice Size	Constituent
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)
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)
AlLi5Si2	(5.3)(0.7)(2)	(Li)(Al)(Si)
AlNi16Si9	(1)(16)(9)	(Al)(Ni)(Si)
AlNi2Si	(1)(1)	(Ni)(Al,Si,Va)

Co10Cu57Ti33	(0.57)(0.1)(0.33)	(Cu)(Co)(Ti)
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)
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)

1.5 Key Elements and Subsystems

The modeling status for the constituent binaries and ternaries of this database are given in Table 1.3 and

Table 1.4. The color represents the following meaning:

: Full description

: Full description for major phases

: Extrapolation

Table 1.3: Modeling status of constituent binary systems

	C	Co	Cr	Cu	Fe	Li	Mg	Mn	Mo	Ni	Si	Ti	V	Zr
Al														
C														
Co														
Cr														
Cu														
Fe														
Li														
Mg														
Mn														
Mo														
Ni														
Si														
Ti														
V														

Table 1.4: Modeling status of constituent ternary systems

	Cr	Cu	Fe	Li	Mg	Mn	Mo	Ni	Si	Ti	V	Zr
Al-Co												
Al-Cr												
Al-Cu												
Al-Fe												
Al-Li												
Al-Mg												
Al-Mn												
Al-Mo												
Al-Ni												
Al-Si												
Al-Ti												
Al-V												
Co-Cr												
Co-Cu												
Co-Fe												
Co-Li												
Co-Mg												
Co-Mn												
Co-Mo												
Co-Ni												
Co-Si												
Co-Ti												
Co-V												
Cr-Cu												
Cr-Fe												
Cr-Li												
Cr-Mg												
Cr-Mn												
Cr-Mo												
Cr-Ni												
Cr-Si												
Cr-Ti												
Cr-V												
Cu-Fe												
Cu-Li												
Cu-Mg												
Cu-Mn												
Cu-Mo												
Cu-Ni												
Cu-Si												
Cu-Ti												
Cu-V												
Fe-Li												
Fe-Mg												
Fe-Mn												
Fe-Mo												
Fe-Ni												
Fe-Si												
Fe-Ti												
Fe-V												
Li-Mg												
Li-Mn												
Li-Mo												
Li-Ni												
Li-Si												
Li-Ti												

	Cr	Cu	Fe	Li	Mg	Mn	Mo	Ni	Si	Ti	V	Zr
Li-V												
Mg-Mn								■				
Mg-Mo												
Mg-Ni									■			
Mg-Si												■
Mg-Ti												
Mg-V												
Mn-Mo								■		■		
Mn-Ni									■	■		
Mn-Si										■		
Mn-Ti											■	■
Mn-V												
Mo-Ni									■	■	■	■
Mo-Si										■	■	■
Mo-Ti											■	■
Mo-V												■
Ni-Si										■	■	■
Ni-Ti											■	■
Ni-V												■
Si-Ti											■	
Si-V												
Ti-V												■

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. Where 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 out experimental studies of $Al_xCoCrFeNi$ alloys [2006Ke, 2008Wan, 2011Kao].

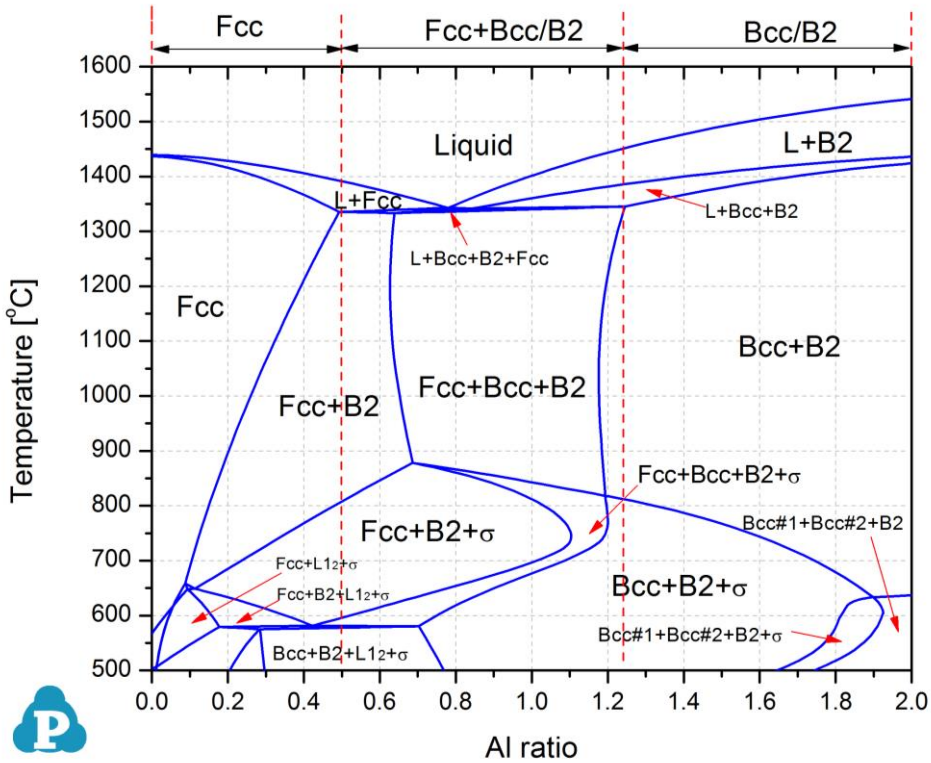


Figure 1.1: Calculated isopleth of the $Al_xCoCrFeNi$ with x=0~2

For quantitative analysis on the phase transformations of an alloy at the given composition, the equilibrium calculation is needed. Figure 14.2 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 $L1_2$_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.

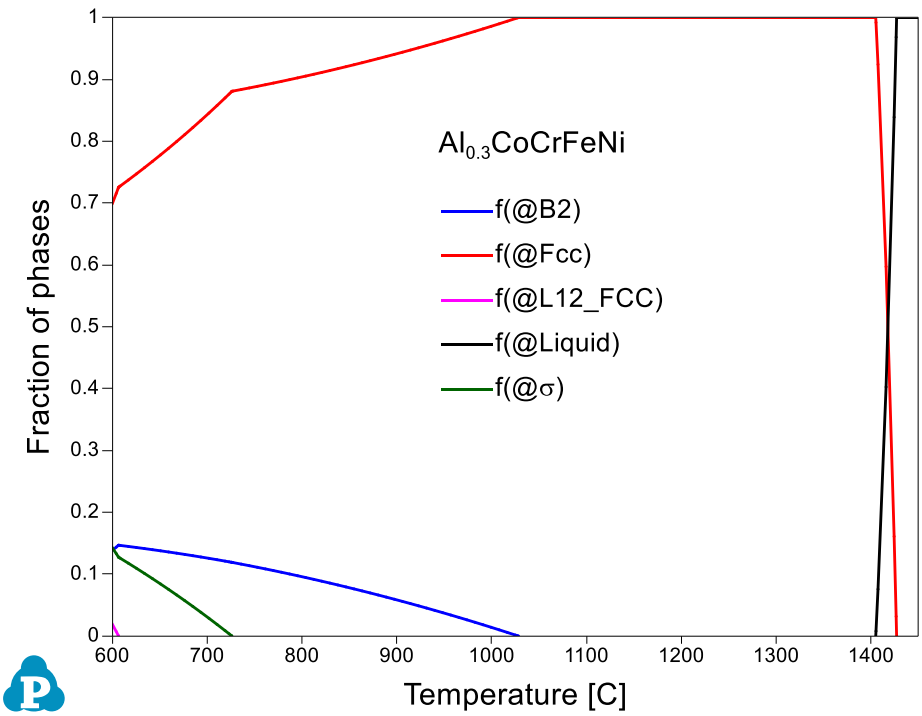


Figure 1.2: Equilibrium calculation of $Al_{0.3}CoCrFeNi$ HEA

1.7 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.

[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.

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