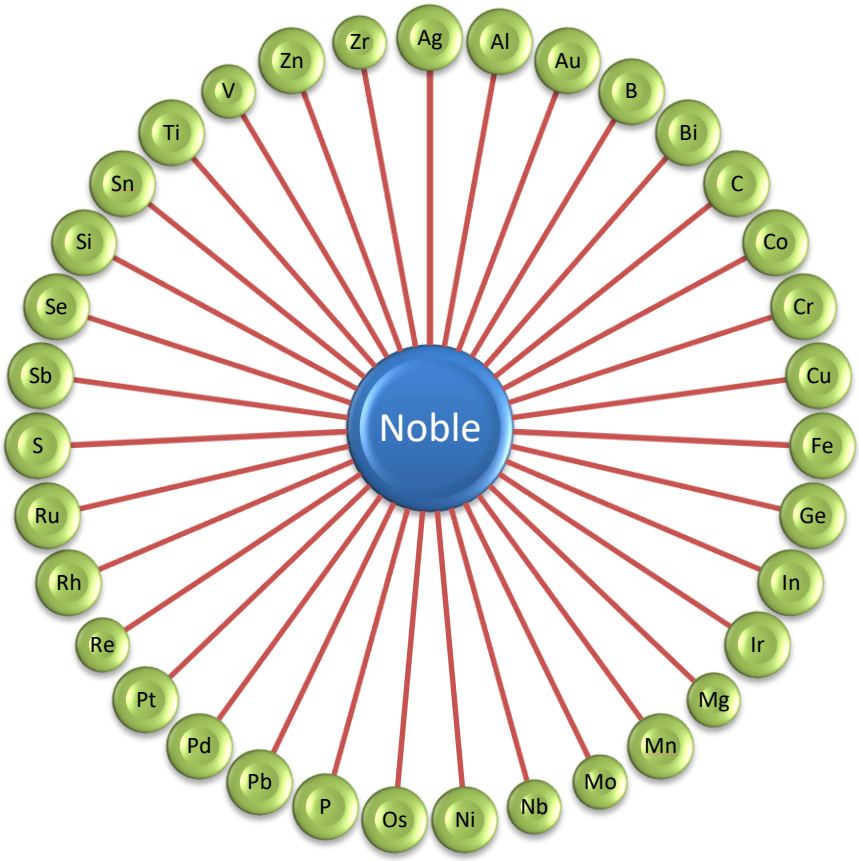
1. PanNoble

Thermodynamic database for multi-component
Noble metal alloys



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1.1 Components

A total of 35 components are included in the database as listed here:

Ag, Al, Au, B, Bi, C, Co, Cr, Cu, Fe, Ge, In, Ir, Mg, Mn, Mo, Nb, Ni, Os, P, Pb, Pd, Pt, Re, Rh, Ru, S, Sb, Se, Si, Sn, Ti, V, Zn and Zr.

1.2 Suggested Composition Range

The suggested composition range for each element is listed in Table 1.1. It should be noted that this given composition range is rather conservative. It is derived from the chemistries of the multicomponent commercial alloys that have been used to validate the current database. In the subsystems, many of these elements can be applied to a much wider composition range. In fact, some subsystems are valid in the entire composition range as given in section 1.4.

Table 1.1: Suggested composition range

Elements	Composition Range (wt.%)
Al, Co, Cr, Cu, Fe, Mn, Ni	0 ~ 100
Bi, In, Pb, Se, Sn, Zn	0 ~ 50
Ag, Au, Ir, Pd, Pt, Sb, Ti	0 ~ 30
Ge, Mg, Mo, Nb, Os, Re, Rh, Ru, Si, V, Zr	0 ~ 10
B, C, P, S	0 ~ 3

1.3 Phases

A total of 863 phases are included in the database and a few key phases are listed in Table 1.2. Information on all the other phases may be displayed through TDB viewer of Pandat or can be found at www.computherm.com.

Table 1.2: Phase name and related information

Name	Lattice Size	Constituent
B2	(1)(1)	(Ag,Al,Co,Cr,Cu,Fe,In,Ir,Mn,Ni,Pd,Ru,Ti,Zn) (Al,Co,Cr,Cu,Fe,Ir,Mn,Ni,Pd,Ru,Zn,Va)
Bcc	(1)(3)	(Ag,Al,Au,B,Bi,Co,Cr,Cu,Fe,Ge,In,Ir,Mn,Ni,Os,P,Pb, Pd,Pt,Rh,Ru,S,Sb,Si,Sn,Ti,Zn)(C,Va)
CBCC_A12	(1)(1)	(Al,Bi,Co,Cr,Cu,Fe,Mn,Ni,Si,Sn,Ti,Zn)(C,Va)
CUB_A13	(1)(1)	(Ag,Al,Bi,Cr,Cu,Co,Fe,Ge,Mn,Ni,Si,Sn,Ti,Zn)(C,Va)
D019	(0.75)(0.25)	(Al,Ni,Sn,Ti)(Al,Ni,Sn,Ti)
Fcc	(1)(1)	(Ag,Al,Au,B,Bi,Co,Cr,Cu,Fe,Ge,In,Ir,Mn,Ni,Os,P,Pb, Pd,Pt,Rh,Ru,S,Sb,Si,Sn,Ti,Zn)(C,Va)
Gamma	(4)(1)(8)	(Ag,Ni,Si,Zn)(Ag,Cu,Ni,Zn)(Cu,Zn)
L12	(0.75)(0.25)	(Al,Co,Cr,Cu,Fe,Ge,Ir,Mn,Ni,Pt,Ru,Si,Ti)(Al,Co,Cr, Cu,Fe,Ge,Ir,Mn,Ni,Pt,Ru,Si,Ti)
Laves_C14	(2)(1)	(Co,Fe,Ti)(Co,Fe,Ti)
Laves_C15	(2)(1)	(Cr,Cu,Fe,Ni,Ti)(Cr,Cu,Fe,Ni,Ti)
Laves_C36	(2)(1)	(Cu,Ni,Ti)(Cu,Ni,Ti)
Liquid	(1)	(Ag,Al,Au,B,Bi,Bi2Se3,C,Co,Cr,CrS,Cr3Ge,CrSe,Cu, Cu2S,Cu2Se,Fe,FeS,FeSe,Ge,Ge3Mn5,In,Ir,Mn,MnS, MnSe,Ni,NiS,Os,P,Pb,PbS,PbSe,Pd,Pt,PtSn,Rh,Ru,S, Sb,Se,SeNi,SeSn,Se2Si,SeZn,Si,Sn,Ti,Zn,ZnS)
Mn5Si3	(2)(3)(3)	(Cr,Fe,Si,Ti)(Cr,Si,Sn,Ti)(Cr,Fe,Ti)
Ni3Sn2	(0.5)(0.25)(0.25)	(Ni,Sn)(Au,Ni)(Au,Ni)
Sigma	(8)(4)(18)	(Al,Co,Fe,Mn,Ni,Ru)(Cr)(Al,Co,Cr,Fe,Mn,Ni,Ru)

1.4 Key Elements and Subsystems

The thermodynamic modeling status for the constituent binaries and ternaries of current 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: Thermodynamic modeling status for the constituent binaries

	Al	Au	B	Bi	C	Co	Cr	Cu	Fe	Ge	In	Ir	Mg	Mn	Mo	Nb	Ni	Os	P	Pb	Pd	Pt	Re	Rh	Ru	S	Sb	Se	Si	Sn	Ti	V	Zn	Zr
Ag																																		
Al																																		
Au																																		
B																																		
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Co																																		
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S																																		
Sb																																		
Se																																		
Si																																		
Sn																																		
Ti																																		
V																																		
Zn																																		

Table 1.4: Thermodynamically modeled constituent ternaries

Ag-Al-Au	Ag-Al-Cu	Ag-Al-Ge	Ag-Al-Si	Ag-Al-Sn	Ag-Al-Zn	Ag-Au-Bi
Ag-Au-Cu	Ag-Au-Ge	Ag-Au-Pb	Ag-Au-Si	Ag-Au-Sn	Ag-Bi-Cu	Ag-Bi-In
Ag-Bi-Pb	Ag-Bi-Sb	Ag-Bi-Sn	Ag-Bi-Zn	Ag-Cu-Ni	Ag-Cu-Ni	Ag-Cu-Pb
Ag-Cu-Zn	Ag-In-Pd	Ag-In-Sb	Ag-In-Sn	Ag-Pb-Sb	Ag-Pb-Sn	Ag-Sb-Sn

Ag-Sn-Zn	Al-Bi-Cu	Al-Bi-Zn	Al-C-Co	Al-C-Mn	Al-C-Ni	Al-Co-Cr
Al-Co-Cu	Al-Co-Fe	Al-Co-Mn	Al-Co-Ni	Al-Cr-Cu	Al-Cr-Fe	Al-Cr-Ni
Al-Cu-Fe	Al-Cu-Mn	Al-Cu-Ni	Al-Cu-Sb	Al-Cu-Si	Al-Cu-Sn	Al-Cu-Zn
Al-Fe-Mn	Al-Fe-Ni	Al-Fe-Si	Al-Fe-Zn	Al-In-Sb	Al-In-Sn	Al-Pb-Zn
Al-Mn-Ni	Al-Si-Sn	Al-Si-Zn	Al-Sn-Zn	Au-Ge-Sb	Au-Ge-Sn	Au-In-Sb
Au-In-Sn	Au-Ni-Sn	Au-Sb-Si	Au-Si-Sn	B-Co-Fe	B-Cu-Fe	B-Fe-Ni
B-Ni-Si	Bi-Cu-Ni	Bi-Cu-Pb	Bi-Cu-Sb	Bi-Cu-Se	Bi-Cu-Sn	Bi-Cu-Zn
Bi-In-Pb	Bi-In-Sb	Bi-In-Sn	Bi-Sb-Sn	Bi-Sb-Zn	Bi-Se-Sn	Bi-Se-Zn
Bi-Sn-Zn	C-Co-Fe	C-Co-Ni	C-Cr-Fe	C-Cu-Fe	C-Fe-Ni	Co-Cr-Cu
Co-Cr-Fe	Co-Cr-Ni	Co-Cu-Fe	Co-Cu-Mn	Co-Cu-Ni	Co-Mn-Ni	Cr-Cu-Fe
Cr-Cu-Mn	Cr-Cu-Ni	Cr-Cu-Si	Cr-Cu-Sn	Cr-Cu-Ti	Cr-Fe-Mn	Cr-Fe-Ni
Cr-Fe-P	Cr-Fe-S	Cr-Fe-Si	Cr-Mn-Ni	Cr-Mn-S	Cr-Ni-S	Cr-Ni-Si
Cu-Fe-Mn	Cu-Fe-Ni	Cu-Fe-P	Cu-Fe-S	Cu-Fe-Sb	Cu-Fe-Si	Cu-Fe-Zn
Cu-In-Sn	Cu-Mn-Ni	Cu-Mn-Zn	Cu-Ni-P	Cu-Ni-Pb	Cu-Ni-Sb	Cu-Ni-Sn
Cu-Ni-Ti	Cu-Ni-Zn	Cu-P-Sn	Cu-Pb-Sb	Cu-Pb-Zn	Cu-S-Pb	Cu-Sb-Se
Cu-Sb-Sn	Cu-Sb-Zn	Cu-Se-Zn	Cu-Si-Ti	Cu-Si-Zn	Cu-Sn-Ti	Cu-Sn-Zn
Cu-Ti-Zn	Fe-Mn-Ni	Fe-Mn-S	Fe-Mn-Si	Fe-Ni-S	Fe-Ni-Si	Fe-Si-Sn
In-Pb-Zn	In-Sb-Sn	In-Sn-Zn	Pb-Sb-Sn	Pb-Sb-Zn	Mn-S-Ni	Ni-Si-Ti
Ni-Si-Zn	Ni-Sn-Zn	Co-Mn-Pd	Cr-Ni-Pd	Co-Fe-Pd	Fe-Ni-Pd	Au-Pt-Re
Co-Fe-Re	Co-Ni-Re	Fe-Ni-Re	Pd-Rh-Ru			

1.5 Database Validation

The current thermodynamic database can be used to calculate the phase diagrams not only for the noble-metal-rich systems (Ag-, Au-, Cu-, Ir-, Pd- and Pt-) but also other common alloying systems, such as Pb and/or Sn-rich solders. Extensive tests and validations have been carried out on the current thermodynamic database using the published experimental data in the literature. A few examples are given below. Figure 1.1 shows the Pt-Sn binary phase diagram with experimental phase boundary data plotted on it. Figure 1.2 shows two isoplethal sections in the of the Ag-Au-Bi ternary system: (a) Ag-Au-85 at.%Bi; (b) Au-Bi-20 at.%Ag. The experimentally measured phase boundary data are also plotted on them for comparison. Figure 1.3 shows comparison between the calculated and measured liquidus temperatures for some Cu-rich alloys.

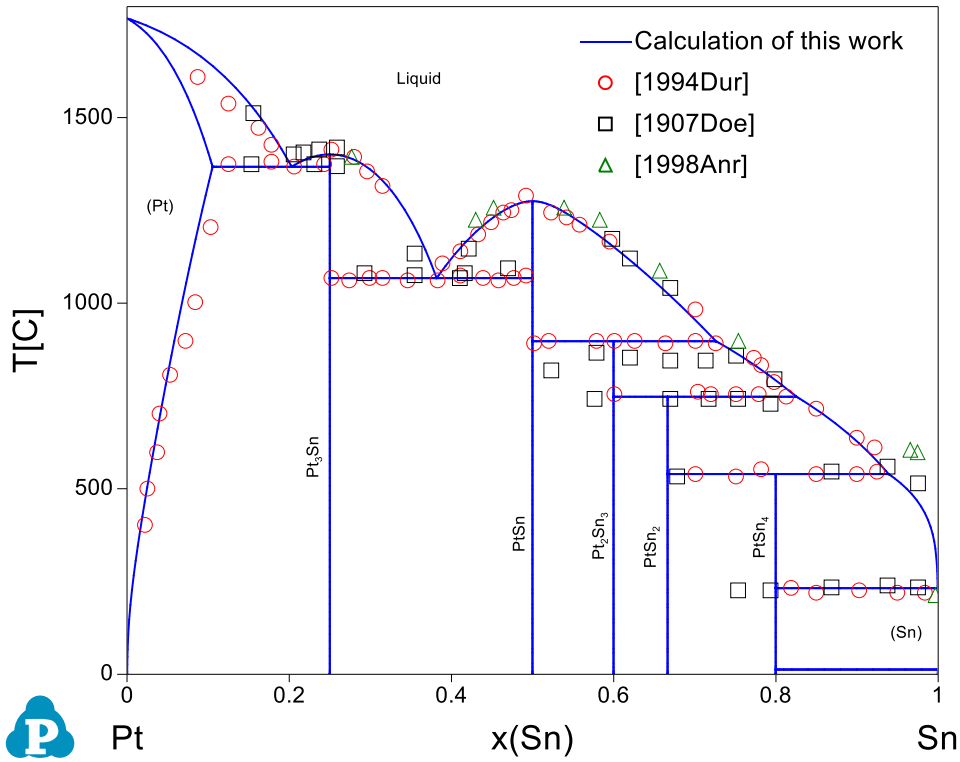
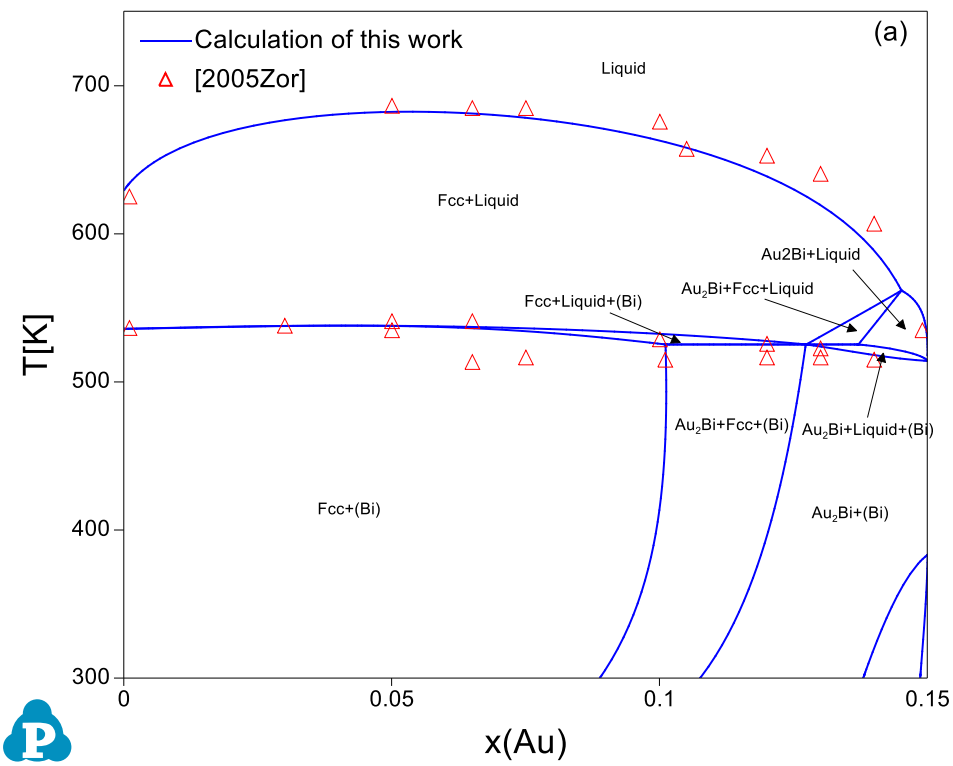


Figure 1.1: Comparison between the calculated Pt-Sn phase diagram with the experimental data



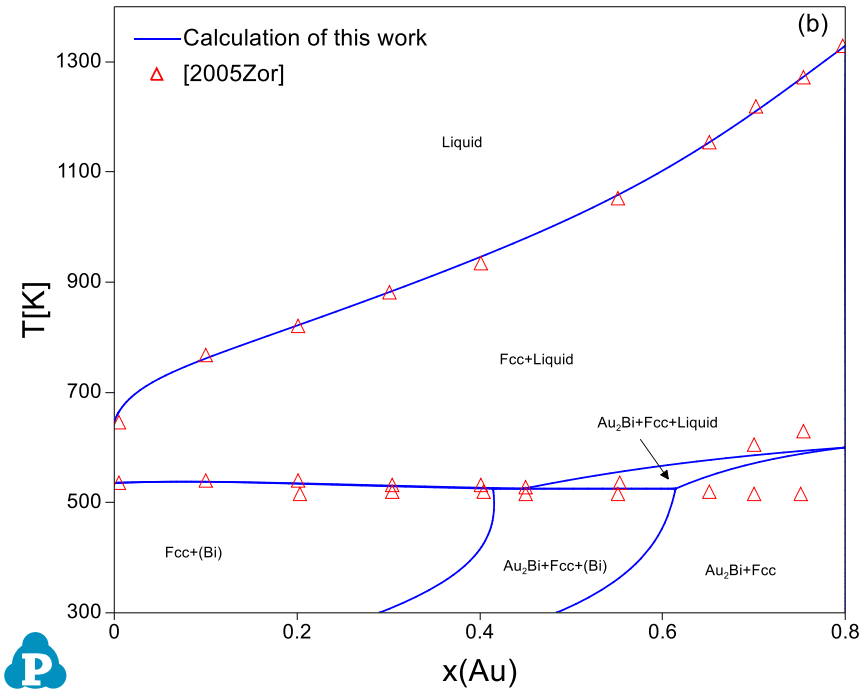


Figure 1.2: Comparison between the calculated isopleths and experimentally measured data of the Ag-Au-Bi ternary system (a) Ag-Au-85 at.%Bi; (b) Au-Bi-20 at.%Ag

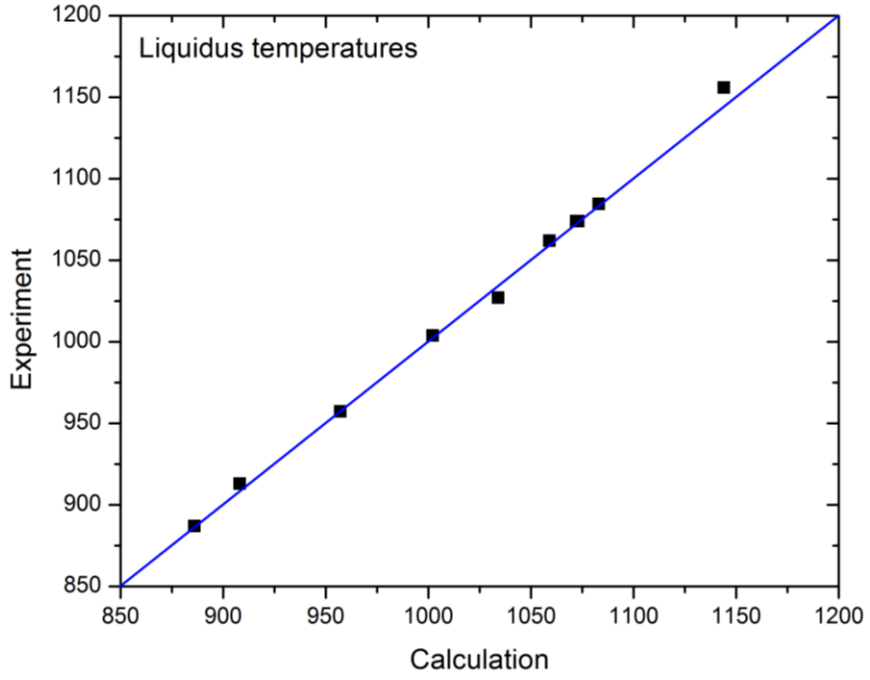


Figure 1.3: Comparison between the calculated and experimentally measured liquidus temperatures of [1982Bac]

Figure 1.4 to Figure 1.8 show the calculated constituent binary phase diagrams, isothermal section and liquidus projection of the Pd-Rh-Ru ternary system.

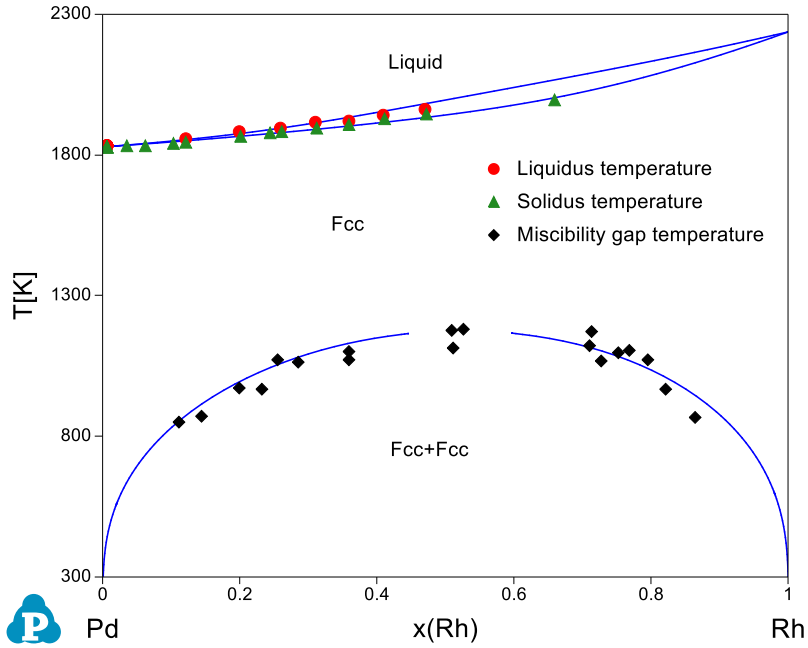


Figure 1.4: Calculated Pd-Rh phase diagram and experimental data from ref. [2016Gos]

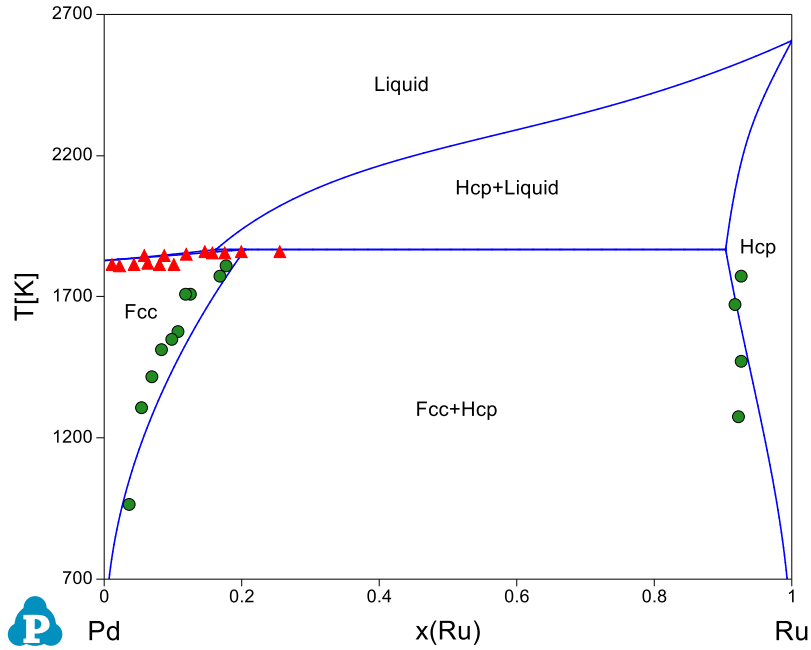


Figure 1.5: Calculated Pd-Ru phase diagram and experimental data from ref. [2016Gos]

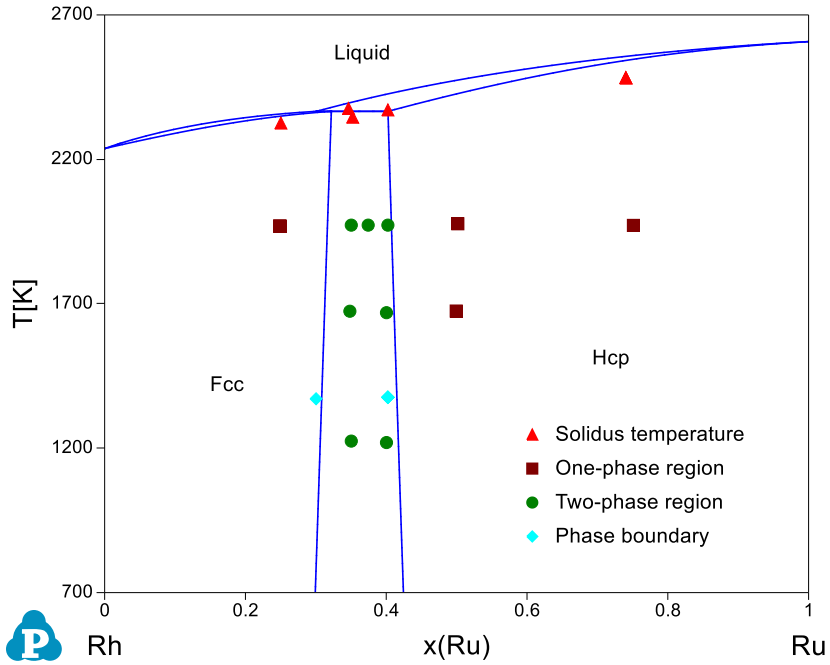


Figure 1.6: Calculated Rh-Ru phase diagram and experimental data from ref. [2016Gos]

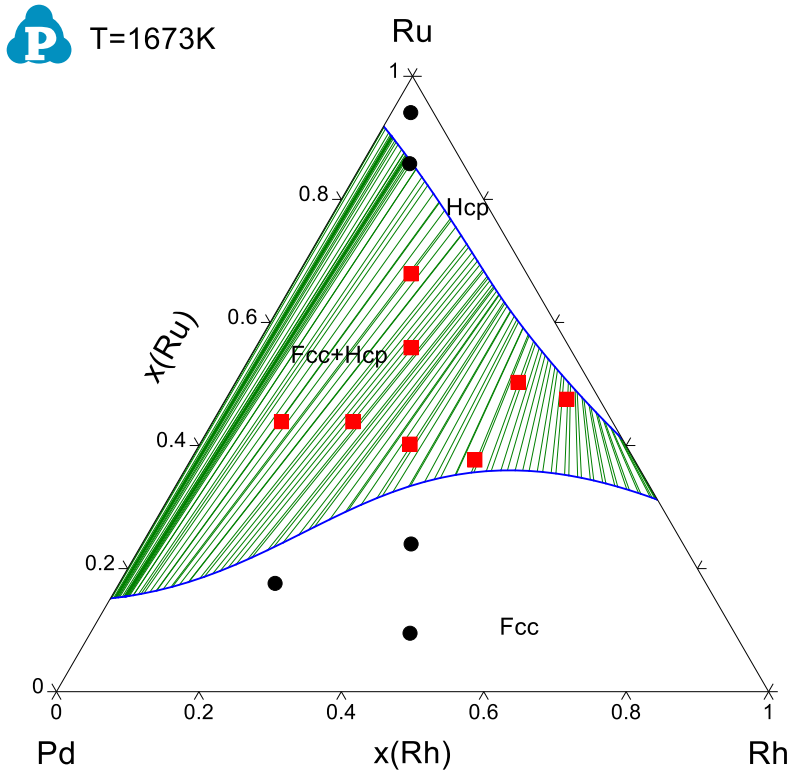


Figure 1.7: Calculated Pd-Rh-Ru isothermal section at 1673K and experimental data from ref. [1984Rae]

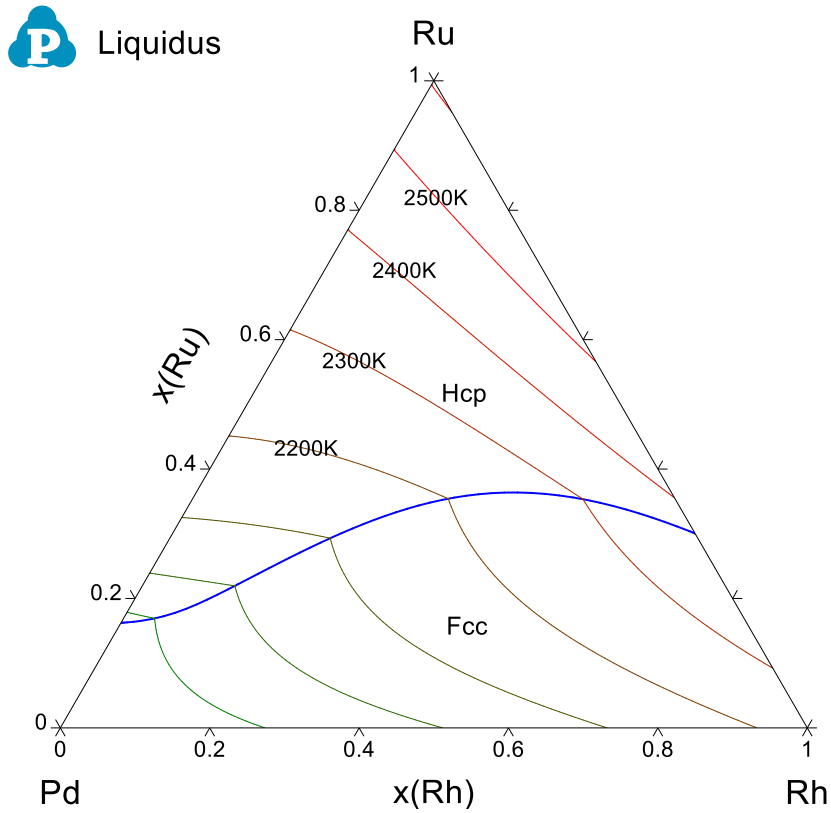


Figure 1.8: Calculated liquidus projection of the Pd-Rh-Ru ternary system

1.6 References

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