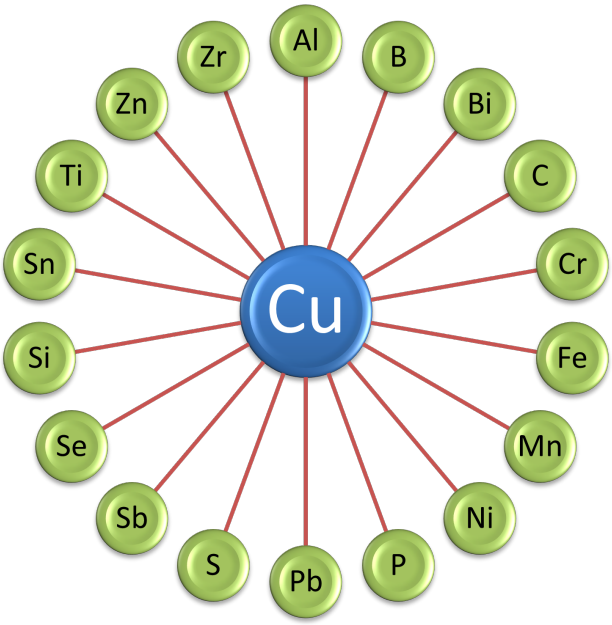
Pandat 2025

Database Manual

CompuTherm LLC

MDT Copper

Database for multi-component Copper-rich alloys



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Contents

1 Thermodynamic Database

1.1 Components (19)

A total of **19** components are included in the database as listed here:

Major alloy elements: **Cu**, Cr, Fe, Mn, Ni, Pb, Si, Sn, Zn

Minor alloy elements: Al, B, Bi, C, P, S, Sb, Se, Ti, 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.%)
Cu	50 ~ 100
Zn	0 ~ 45
Ni	0 ~ 35
Sn	0 ~ 14
Cr, Fe, Mn	0 ~ 10
Pb, Si	0 ~ 5
Al, Sb	0 ~ 3
Bi, P, Se, Zr	0 ~ 2
B, C, S, Ti	0 ~ 0.5

1.3 Phases

A total of **330** 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.

Table 1.2: Phase name and related information

Name	Lattice Size	Constituent
Ag5Zn8	(0.667)(0.333)	(Al)(Al,Cu)
AlCu_Delta	(0.4)(0.6)	(Al)(Cu)
AlCu_Eps1	(0.4)(0.6)	(Al,Cu)(Al,Cu)
AlCu_Eps2	(0.5)(0.5)	(Al,Cu)(Cu)
AlCu_Eta	(0.5)(0.5)	(Al,Cu)(Cu)
AlCu_Zeta	(0.45)(0.55)	(Al)(Cu)
Bcc	(1)(3)	(Al,B,Bi,Cr,Cu,Fe,Mn,Ni,P,Pb,Si,Sn,Ti,Zn) (C,Va)
Cu4Ti	(0.8)(0.2)	(Cu,Ti)(Cu,Ti)
Cu4Ti3	(0.571)(0.429)	(Cu)(Ti)
Cu56Si11	(0.835821) (0.164179)	(Cu,Zn)(Si)

Name	Lattice Size	Constituent
CuInSn_Eta	(0.545)(0.122) (0.333)	(Cu)(Cu,Sn)(Sn)
Fcc	(1)(1)	(Al,B,Bi,Cr,Cu,Fe,Mn,Ni,P,Pb,Si,Sn,Ti,Zn) (C,Va)
Gammabrass	(1)	(Al,Cu,Fe,Ni,Si,Zn)
Hcp	(1)(0.5)	(Al,B,Bi,Cr,Cu,Fe,Mn,Ni,Pb,Si,Sn,Ti,Zn) (C,Va)
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)	(Al,B,Bi,Bi2Se3,C,Cr,CrSe,Cu,Cu2Se, Fe,FeSe,Mn,Ni,P,Pb,Se,MnSe,PbSe, Si,Sn,SeNi,SeSn,Se2Si,SeZn,Ti,Zn)

1.4 Key Elements and Subsystems

Key elements of the system are listed as: **Cu**-Cr-Fe-Mn-Ni-Pb-Si-Sn-Zn. The modeling status for all the constituent binaries and key ternaries are given in The color represents the following meaning:

: Full description

: Full description for major phases

: Extrapolation

Table 1.3: Modeling status of constituent binary systems

	B	Bi	C	Cr	Cu	Fe	Mn	Ni	P	Pb	S	Sb	Se	Si	Sn	Ti	Zn	Zr
Al																		
B																		
Bi																		
C																		
Cr																		
Cu																		
Fe																		
Mn																		
Ni																		
P																		
Pb																		
S																		
Sb																		
Se																		
Si																		
Sn																		
Ti																		
Zn																		

Table 1.4: Modeling status of constituent ternary systems

Al-Cu-Fe	Al-Cu-Ni	Al-Cu-Sb	Al-Cu-Si	Al-Si-Zn	B-Ni-Si	Bi-Cu-Ni	Bi-Cu-Pb
Bi-Cu-Sn	Bi-Cu-Zn	Bi-Cu-Se	Bi-Se-Zn	Bi-Sn-Zn	C-Cr-Fe	C-Cu-Fe	Cr-Cu-Ni
Cr-Cu-Si	Cr-Cu-	Cr-Cu-Ti	Cr-Fe-Ni	Cr-Fe-S	Cr-Mn-S	Cr-Ni-Si	Cu-Fe-S
Cu-Fe-Ni	Cu-Fe-	Cu-Fe-Si	Cu-Fe-	Cu-Mn-	Cu-Mn-	Cu-Se-	Cu-Ni-P
Cu-Ni-Si	Cu-Ni-	Cu-Ni-Ti	Cu-Ni-Zn	Cu-P-Sn	Cu-Pb-	Cu-Sb-	Cu-Pb-S
Cu-Sb-	Cu-Sb-	Cu-Si-Zn	Cu-Sn-Ti	Cu-Sn-	Cu-Ti-Zn	Fe-Mn-	Fe-Mn-S
Fe-Ni-S	Ni-Si-Ti						

1.5 Database Validation

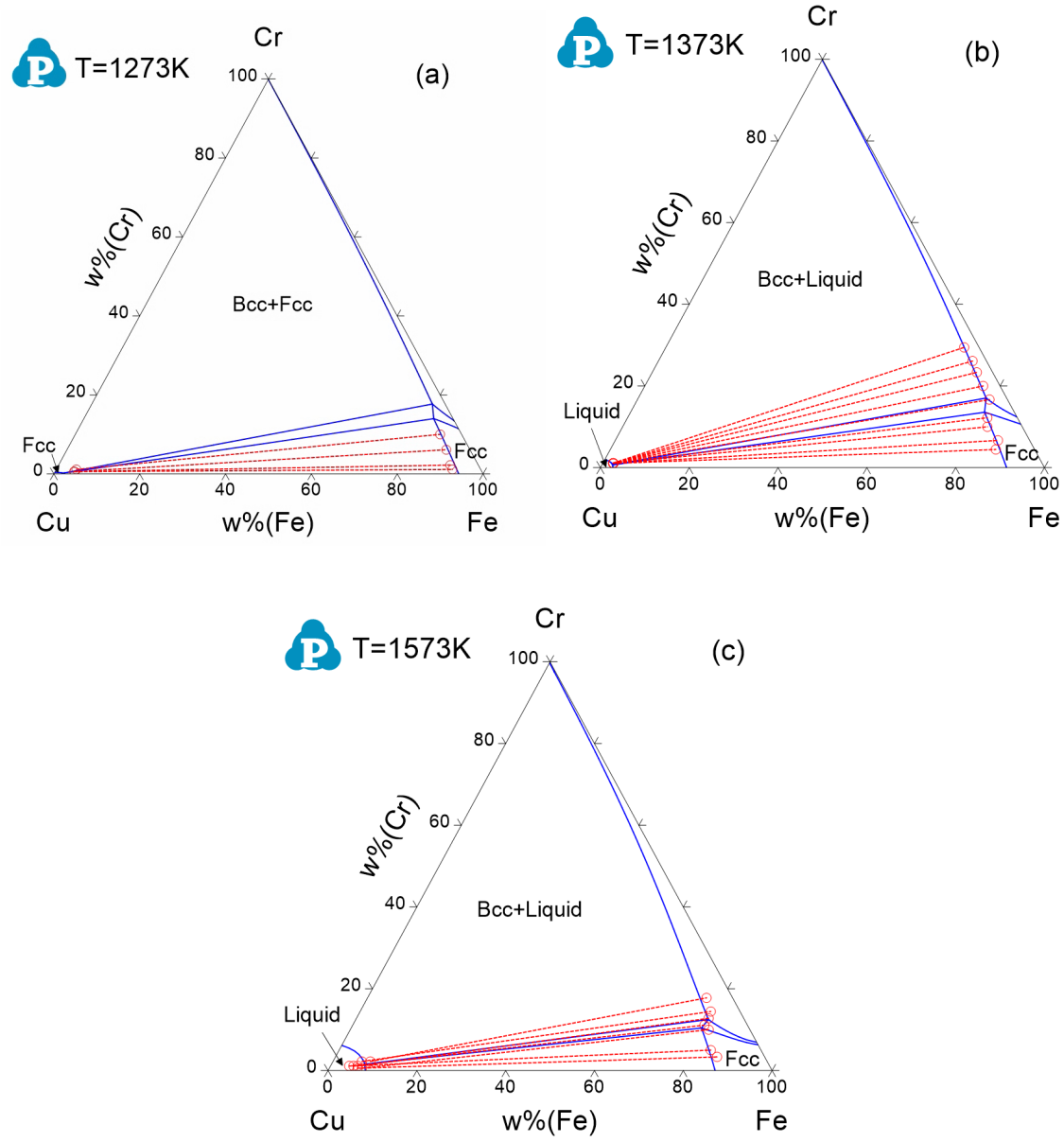

Figure 1.1: Calculated isothermal section diagrams of the Fe-Cu-Cr system at (a) 1273K, (b) 1373K, and (c) 1573K with the experimental data [1997Oht, 2002Wan]

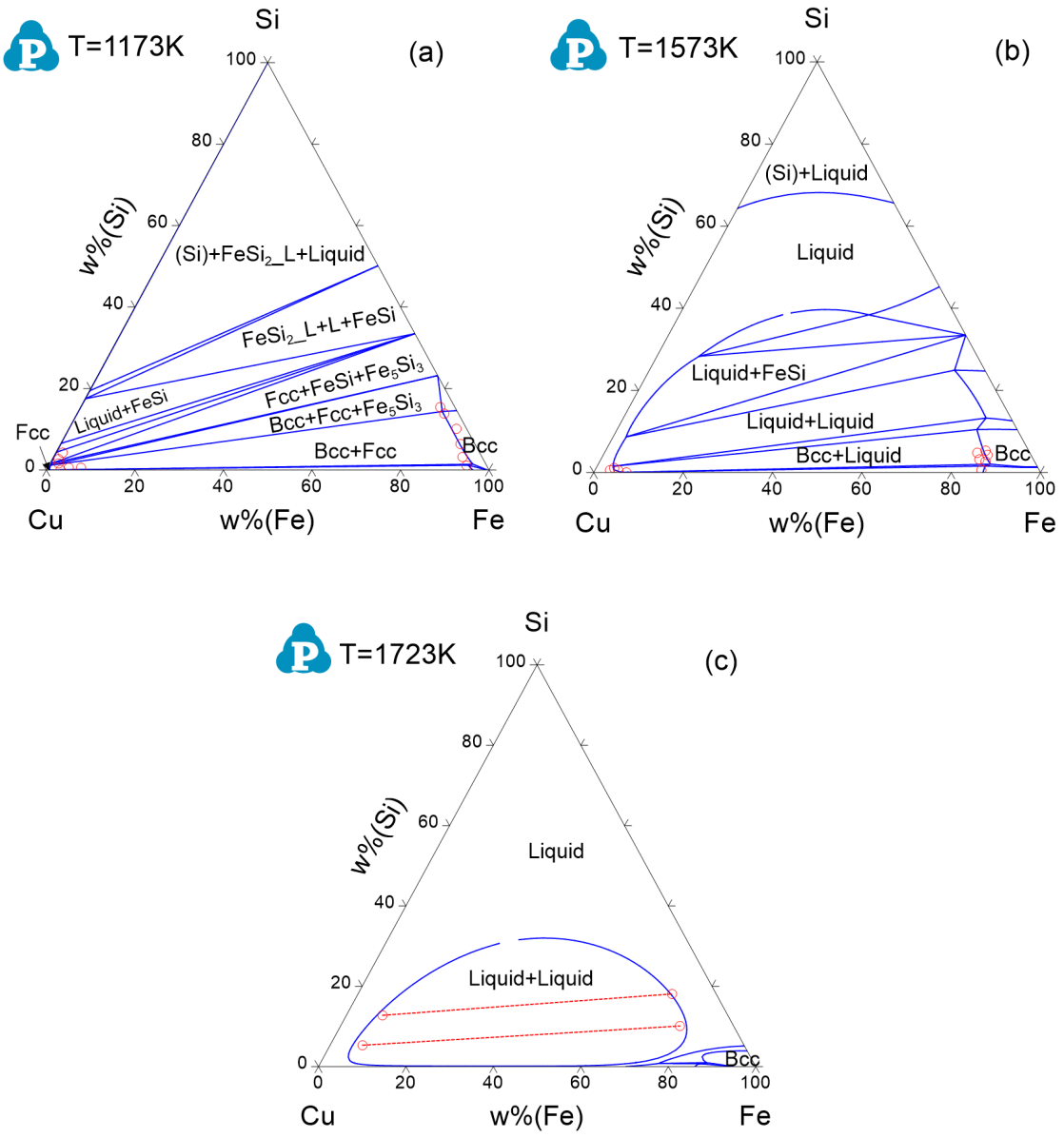

Figure 1.2: Calculated isothermal section diagrams of the Fe-Cu-Si system at (a) 1173K, (b) 1573K, and (c) 1723K with the experimental data [1997Oht, 1999Him, 2002Wan]

2 Mobility Database

PanCu2025_MB is an atomic mobility database for Cu-based alloys, which is compatible with the MDTCu2025_TH thermodynamic database and suitable for the simulation of diffusion-controlled phenomena using the PanDiffusion module, PanEvolution module, and/or PanSolidification module.

2.1 Components (19)

Al	B	Bi	C	Cr	Cu	Fe	Mn	Ni	P
Pb	S	Sb	Se	Si	Sn	Ti	Zn	Zr	

2.2 Phases

The atomic mobility within the Liquid, Bcc, Fcc, and Hcp solution phases are assessed in this database.

2.3 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	Bi	Cr	Cu	Fe	Mn	Ni	Pb	Sb	Si	Sn	Ti	Zn	Zr
Bcc														
Fcc														
Hcp														

2.4 Assessed Systems

In addition to the assessed self-diffusivities shown above, the impurity diffusion data for all included elements in the current PanCu2025_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-Cu	Al-Ni	Al-Si	Al-Zn	Cr-Fe	Cr-Ni	Cu-Fe	Cu-Si	Cu-Sn	Cu-Ti
Cu-Zn	Fe-Mn	Fe-Ni	Fe-Si	Mn-Ni	Ni-Ti	Ni-Zn			

Al-Cr-Ni	Al-Cu-Si	Al-Cu-Zn	Al-Mn-Ni	Cr-Cu-Ni	Cr-Fe-Ni
Cu-Fe-Mn	Cu-Fe-Ni	Cu-Mn-Ni	Cu-Ni-Zn	Fe-Mn-Si	

Bcc phase

Al-Fe	Al-Ti	Cr-Fe	Cr-Ti	Cu-Ti	Fe-Ti	Ti-Zr			

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

2.5 Database Validation

The simulated concentration profiles of a series of Cu-based alloys are used to validate the current mobility database for Cu-based alloys. A few examples of such simulation are shown below.

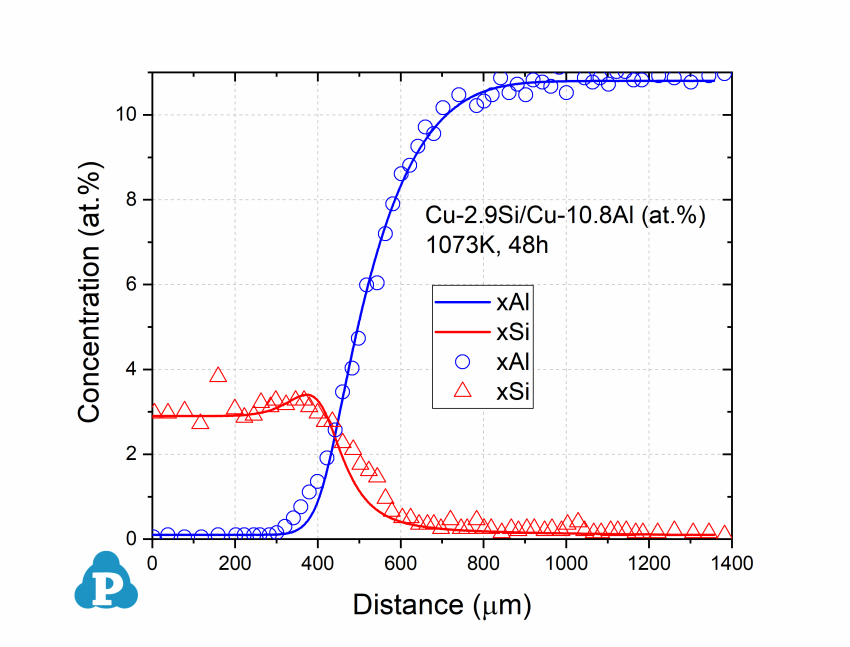

Figure 2.1: Concentration profiles of Cu2.9Si-Cu10.8Al (at.%) at 1073K for 48h [2013Liu]

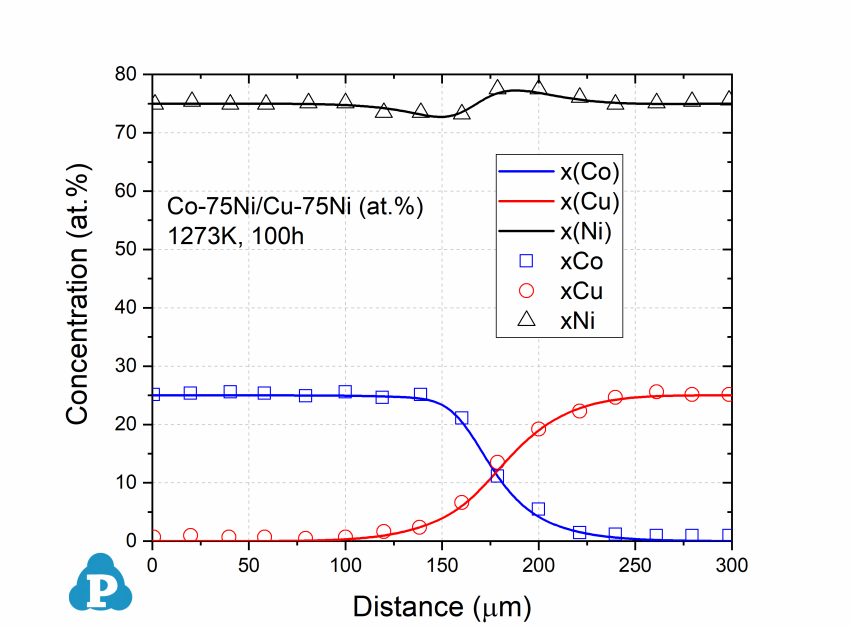

Figure 2.2: Concentration profiles of Co75Ni-Cu75Ni (at%) at 1273K for 100h [2014Che]

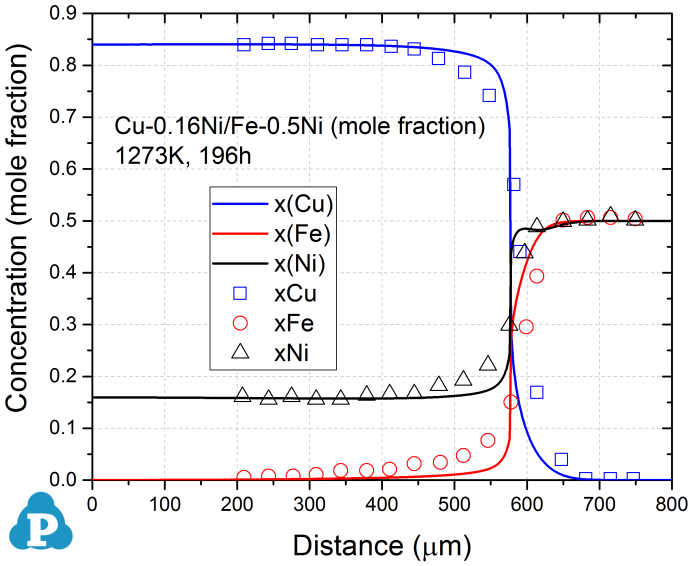

Figure 2.3: Concentration profiles of Cu-0.16Ni/Fe-0.5Ni (mole fraction) at 1273K for 196h [2011Liu]

3 Molar Volume Database

PanCu2025_MV is a molar volume database for Cu-based alloys, which is compatible with the `MDTCu2025_TH` thermodynamic database and suitable for the simulation of thermophysical properties of Cu-based alloys, such as density, thermal expansion, solidification shrinkage etc.

3.1 Components (19)

Al	B	Bi	C	Cr	Cu	Fe	Mn	Ni	P
Pb	S	Sb	Se	Si	Sn	Ti	Zn	Zr	

3.2 Phases

The current molar volume database covers all 330 phases assessed in the `MDTCu2025_TH` database

3.3 Database Validation

The simulated density changes vs. temperature of a series of Cu-based alloys are shown below to validate the current PanCu2025_MV database.

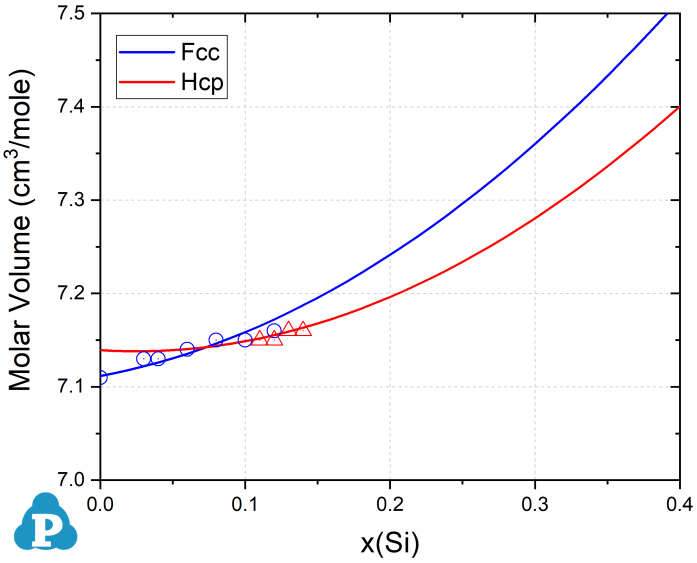

Figure 3.1: Molar volume of Cu-Si Fcc and Hcp binary alloys at 298K [2006Hal]

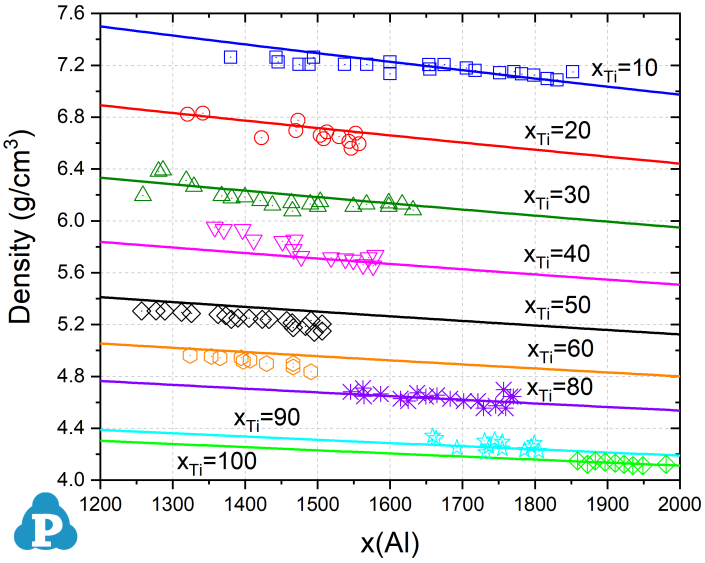

Figure 3.2: Density of Cu-Ti binary liquid mixture [2013Amo]

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