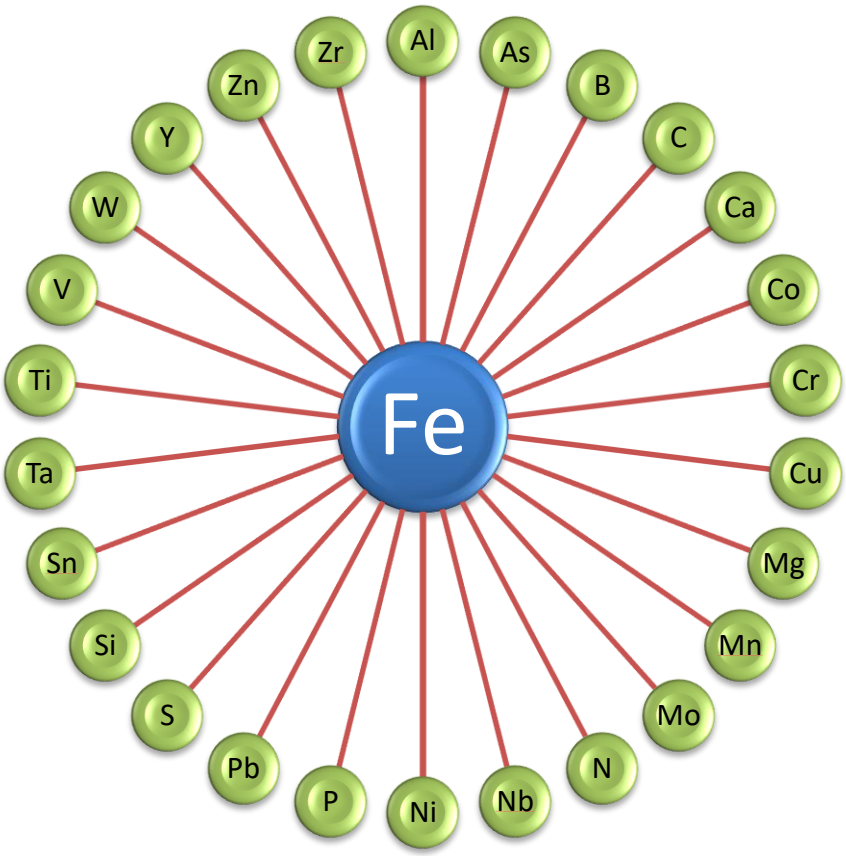
1. PanIron

Thermodynamic database for multi-component
Fe-rich alloys



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1.1 Components

Total of 27 components are included in the database as listed here:

Major alloy elements: Co, Cr, Fe, Mo, Ni, V and W.

Minor alloy elements: Al, As, B, C, Ca, Cu, Mg, Mn, N, Nb, P, Pb, S, Si, Sn, Ta, Ti, Y, 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.%)
Fe	50 ~ 100
Cr, Ni	0 ~ 34
Mn	0 ~ 15
Al, Co, Mo	0 ~ 10
Pb, V, W	0 ~ 7
B, C, Cu, Nb, Si, Ti	0 ~ 5
As, Ca, Mg, N,	0 ~ 0.5
P, S, Sn, Ta,Y,Zn,Zr	0 ~ 0.1

1.3 Phases

Total of 534 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 may 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
Bcc(ferrite)	(1)(3)	(Al,As,Ca,Co,Cr,Cu,Fe,Mg,Mn,Mo,Nb,Ni,P,Pb,S, Si,Sn,Ta,Ti,V,W,Y,Zn,Zr)(B,C,N,Va)
Cementite	(3)(1)	(Co,Cr,Fe,Mn,Mo,Nb,Ni,V,W)(B,C,N)
Fcc(austenite)	(1)(1)	(Al,As,Ca,Co,Cr,Cu,Fe,Mg,Mn,Mo,Nb,Ni,P,Pb,S, Si,Sn,Ta,Ti,V,W,Y,Zn,Zr)(B,C,N,Va)
Graphite	(1)	(B,C)
Laves_C14	(2)(1)	(Al,Co,Cr,Fe,Mg,Mn,Mo,Nb,Ni,Ti,W,Zn,Zr) (Al,Co,Cr,Fe,Mg,Mn,Mo,Nb,Ni,Ti,W,Zn,Zr)
M23C6	(20)(3)(6)	(Co,Cr,Fe,Mn,Ni,V)(Co,Cr,Fe,Mn,Mo,Ni,V,W) (B,C)
M3C2	(3)(2)	(Co,Cr,Mo,V,W)(C)
M5C2	(5)(2)	(Fe,Mn,V)(C)
M6C	(2)(2)(2)(1)	(Co,Fe,Ni)(Cr,Mo,Nb,W) (Co,Cr,Fe,Mo,Nb,Ni,Si,V,W)(C)
M7C3	(7)(3)	(Co,Cr,Fe,Mn,Mo,Ni,V,W)(C)
Mu_PHASE	(7)(2)(4)	(Al,Co,Cr,Fe,Mo,Mn,Nb,Ni,Ta)(Mo,Nb,Ta,W) (Al,Co,Cr,Fe,Mo,Nb,Ni,Ta,W)
Sigma	(8)(4)(18)	(Al,Co,Cr,Fe,Mn,Ni,Si,Ta)(Cr,Fe,Mo,Nb,Ta,Ti,V, W)(Al,Co,Cr,Fe,Mn,Mo,Nb,Ni,Si,Ta,Ti,V,W)

1.4 Key Elements and Subsystems

The modeling status for the constituent binaries and ternaries 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

	As	B	C	Ca	Co	Cr	Cu	Fe	Mg	Mn	Mo	N	Nb	Ni	P	Pb	S	Si	Sn	Ta	Ti	V	W	Y	Zn	Zr
Al																										
As																										
B																										
C																										
Ca																										
Co																										
Cr																										
Cu																										
Fe																										
Mg																										
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Pb																										
S																										
Si																										
Sn																										
Ta																										
Ti																										
V																										
W																										
Y																										
Zn																										

Table 1.4: Key ternary systems for the major components

	Co	Si	Cr	Mo	Ni	W
Fe-B	Fe-B-Co	Fe-B-Si	Fe-B-Cr	Fe-B-Mo	Fe-B-Ni	Fe-B-W
Fe-C	Fe-C-Co	Fe-C-Si	Fe-C-Cr	Fe-C-Mo	Fe-C-Ni	Fe-C-W
Fe-Co			Fe-Co-Cr	Fe-Co-Mo	Fe-Co-Ni	Fe-Co-W
Fe-Cr				Fe-Cr-Mo	Fe-Cr-Ni	Fe-Cr-W
Fe-Mo					Fe-Mo-Ni	Fe-Mo-W
Fe-Ni						Fe-Ni-W

1.5 Database Validation

The current thermodynamic database for iron-based alloy systems has been extensively tested and validated using the published experimental data. This database can be used to calculate phase equilibria for multi-component iron

alloys, such as the equilibrium between Bcc (ferrite) and Fcc (austenite). It can be used to predict phase transformation temperatures, such as liquidus, solidus, and so on. The fraction of each phase as a function of temperature, partitioning of components in different phases can also be calculated. In addition to equilibrium calculations, Scheil simulations can also be carried out using this database. Some validation results are presented below. Figure 1.1 shows comparison between the calculated and experimentally measured liquidus and solidus temperatures for variety of steels. Figure 1.2 shows comparison between the calculated and experimentally observed amounts of austenite in duplex stainless steels. Figure 1.3 is a comparison between the calculated and experimentally measured partitioning of Fe, Cr, Mo, and Ni in ferrite and austenite. Figure 1.4 ~ Figure 1.8 are comparisons between the calculated and experimentally observed equilibrium compositions for Fe, C, Co, Cr, Mo, Si, V and W in austenite, ferrite, M_6C, MC and M_2C at 1200^oC, respectively. These figures show reasonable agreement between the calculated values using the current PanFe database and the experimental determined ones.

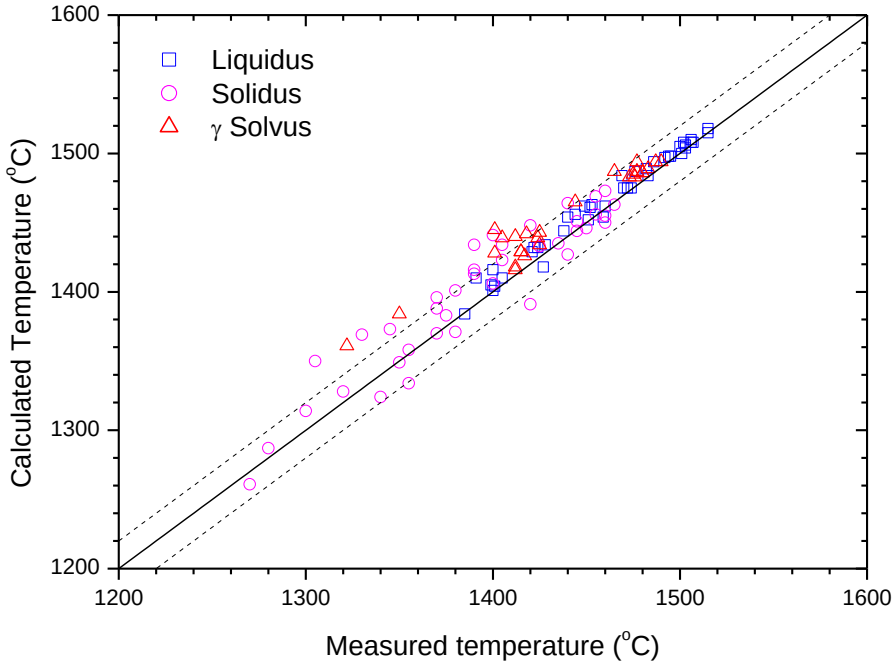

Figure 1.1: Comparison between the calculated liquidus and solidus temperatures for iron-based alloys with experimental data from [1977Jer]

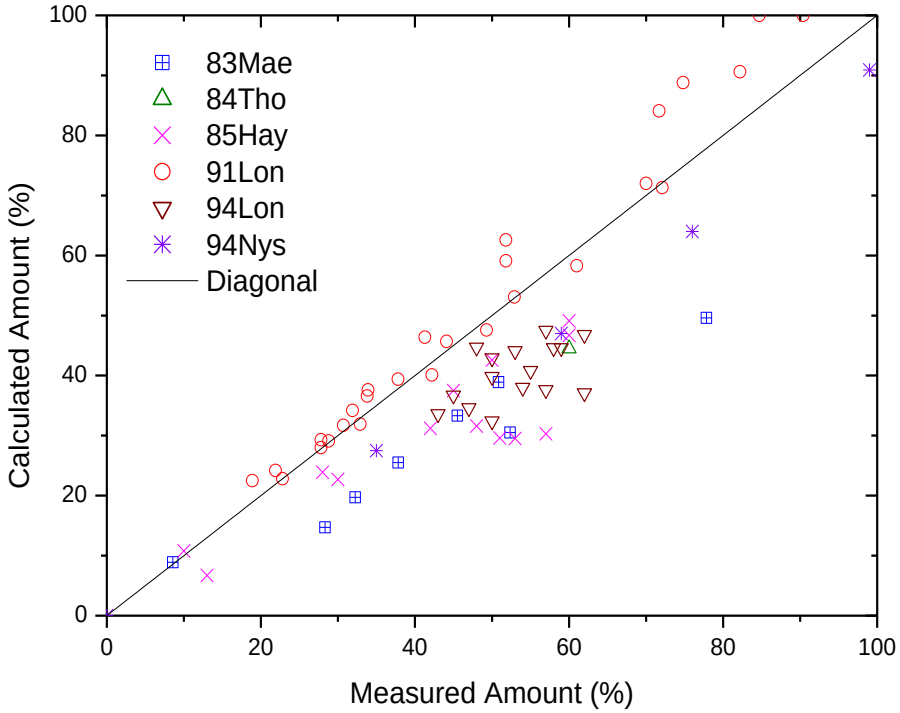

Figure 1.2: Comparison between the calculated and experimentally measured amounts of austenite in duplex stainless steels of austenite (Fcc)

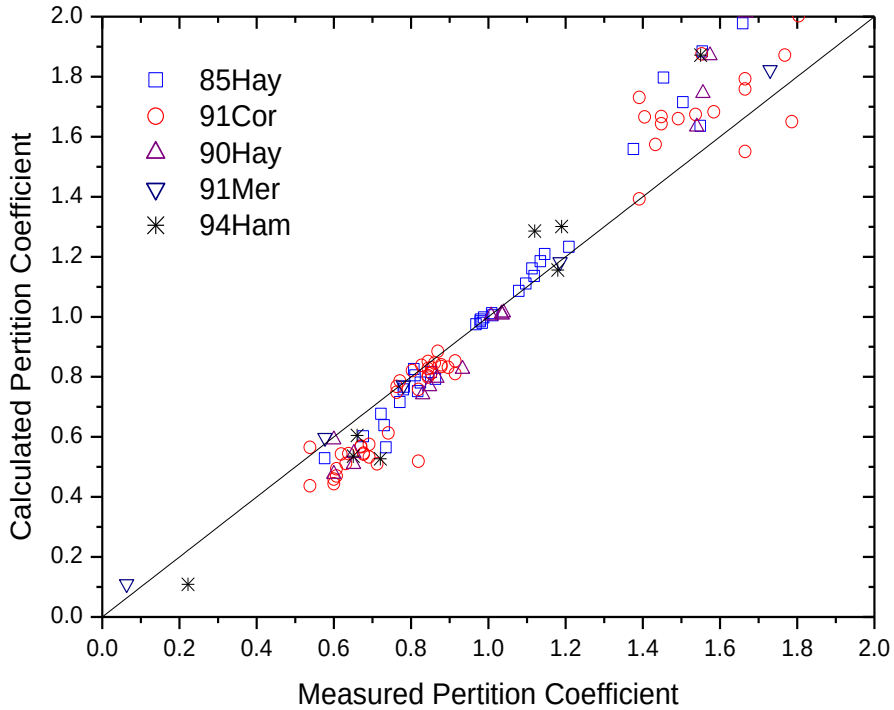

Figure 1.3: Comparison between the calculated and experimentally measured partitioning of Fe, Cr, Mo and Ni in ferrite and austenite

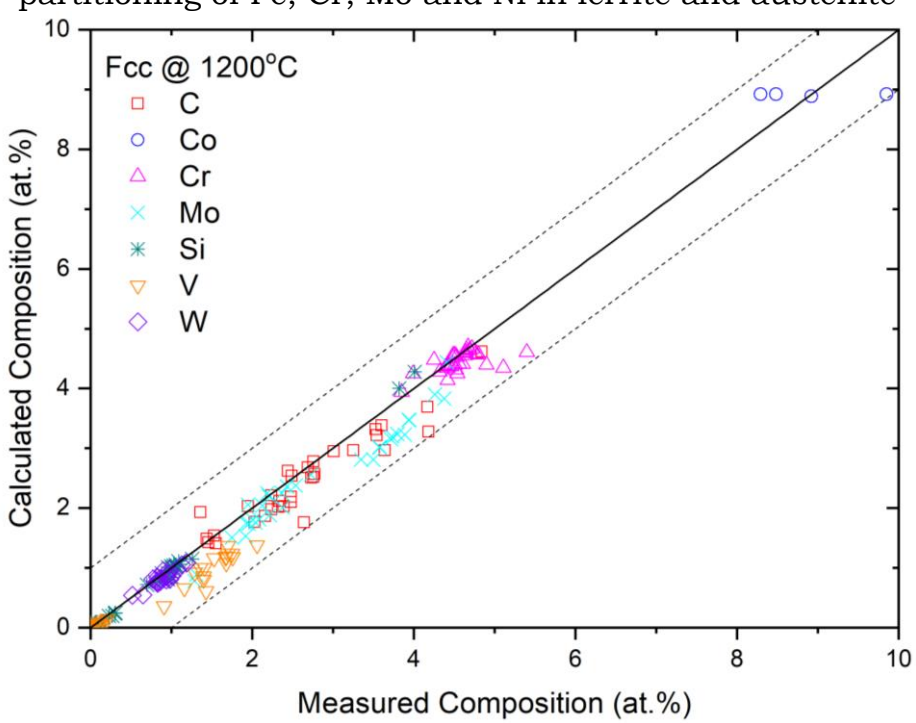

Figure 1.4: Comparison between the calculated and measured equilibrium compositions of C, Co, Cr, Mo, Si, V and W in the Fcc phase at 1200°C

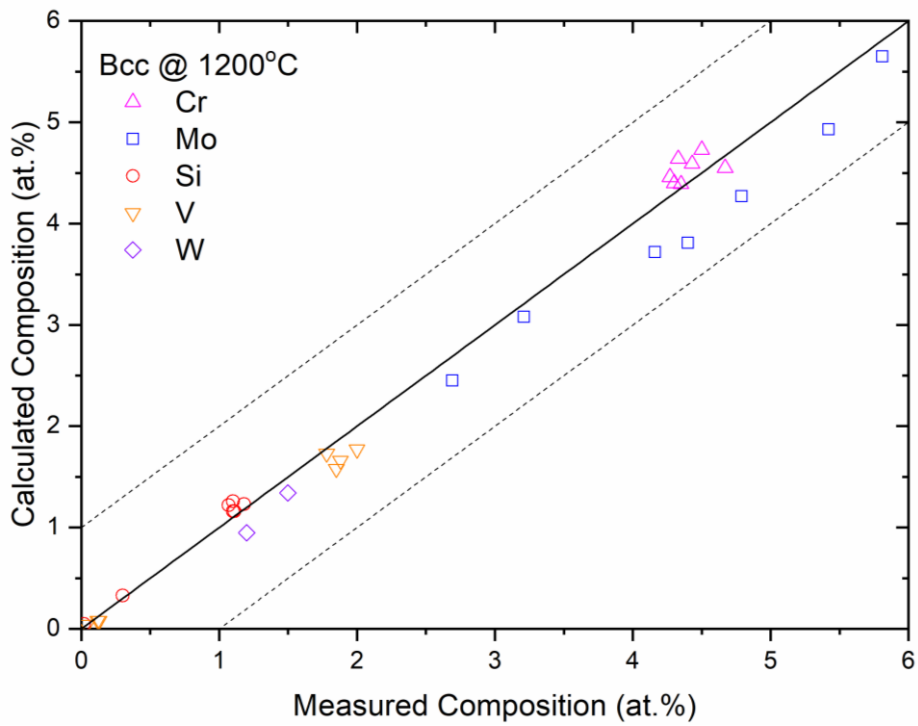

Figure 1.5: Comparison between the calculated and measured equilibrium compositions of Cr, Mo, Si, V and W in the Bcc (ferrite) phase at 1200°C

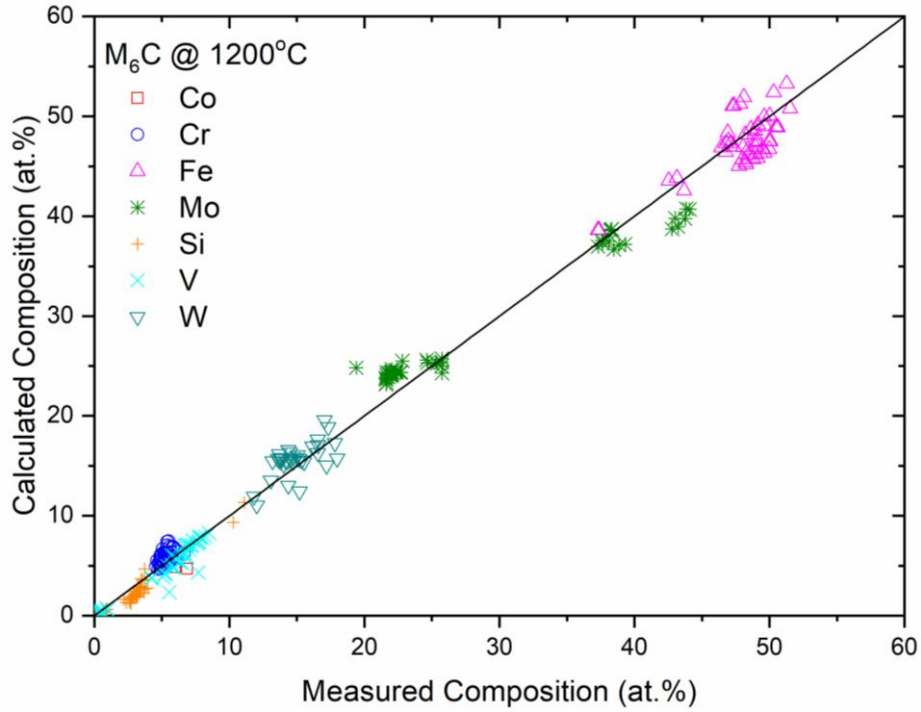

Figure 1.6: Comparison between the calculated and measured equilibrium compositions of Cr, Mo, Fe, V and W in the M_6C phase at 1200°C

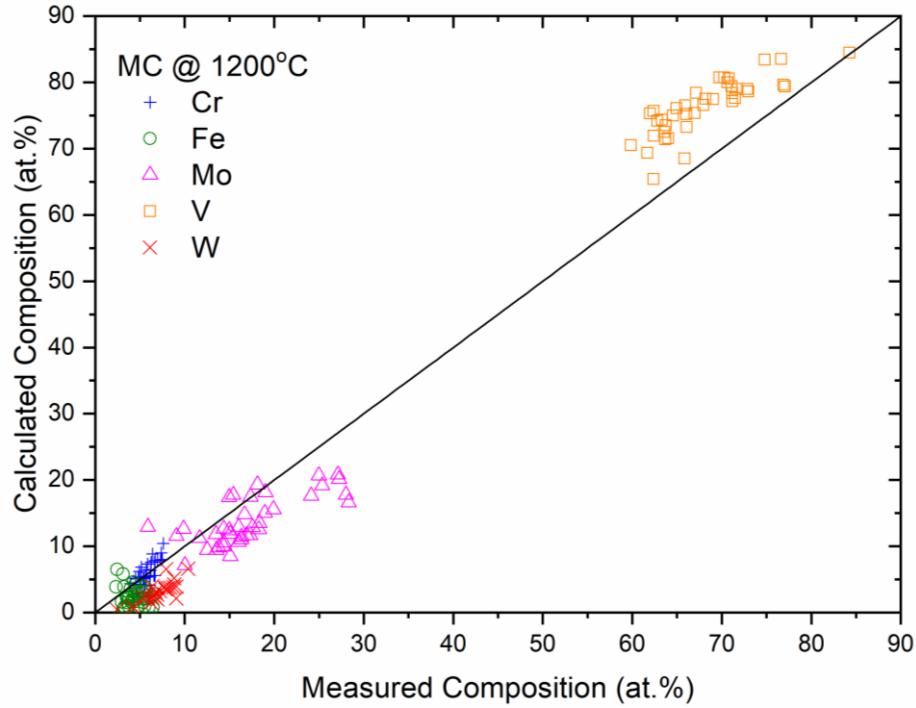

Figure 1.7: Comparison between the calculated and measured equilibrium compositions of Cr, Fe, Mo, V and W in the MC phase at 1200°C

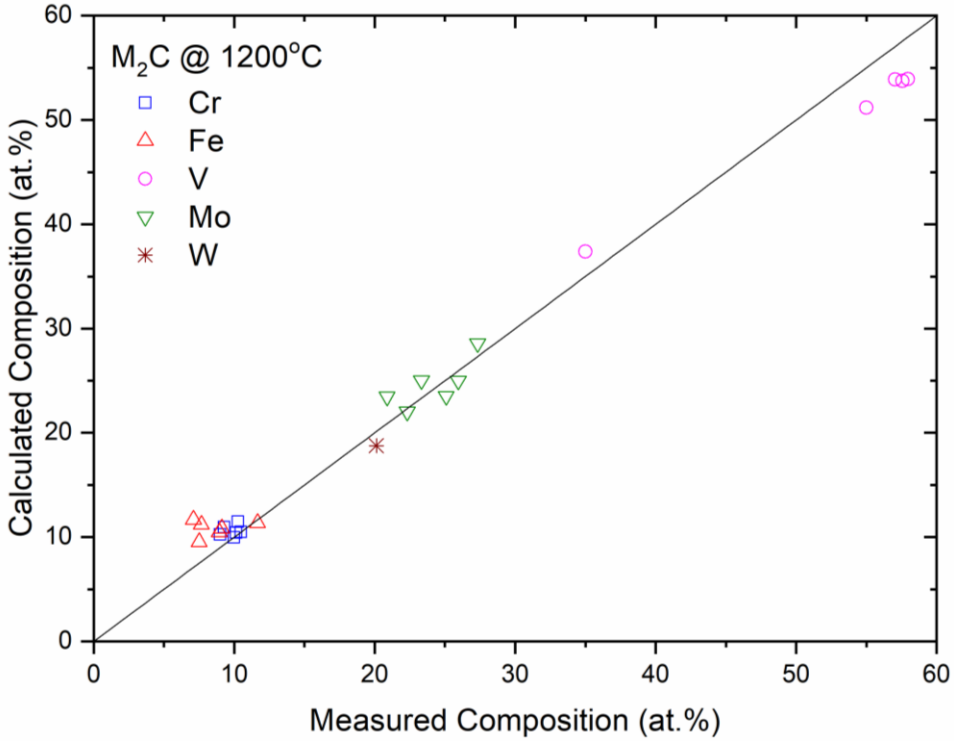

Figure 1.8: Comparison between the calculated and measured equilibrium compositions of Cr, Fe, Mo, V and W in the M_2C (Hcp) phase at 1200°C

1.6 References

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