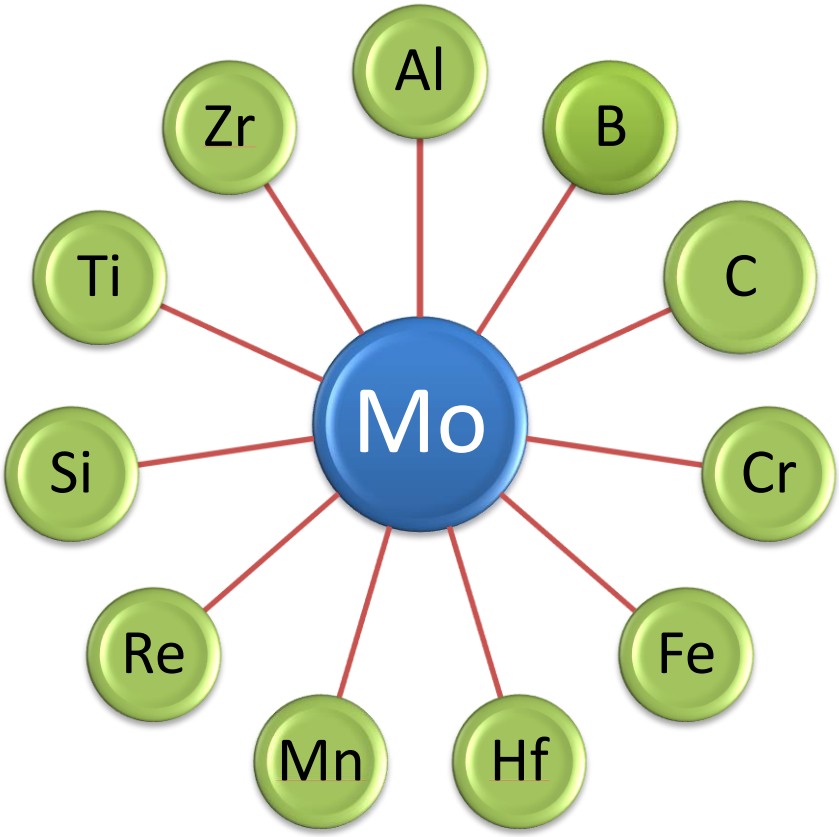
1. PanMolybdenum

Thermodynamic database for multi-component
Mo-rich alloys



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1.1 Components

Total of 12 components are included in the database as listed here:

Major alloying elements Al, B, Cr, Hf, Mn, **Mo**, Re, Si, Ti

Minor alloying elements: C, Fe, 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

Element	Composition range (at.%)
Mo	50 ~ 100
Si, Ti	0 ~ 30
B, Cr	0 ~ 20
Al, Hf, Mn, Re	0 ~ 10
C, Fe, Zr	0 ~ 5

1.3 Phases

Total of 168 phases are included in the database and a few key phases are listed in Table 1.2. Information on all the 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
Al12Mo	(0.923)(0.077)	(Al)(Mo)
Al4Mo3Ti3	(4)(3)(3)	(Al)(Mo)(Ti)
Al63Mo37	(0.63)(0.37)	(Al)(Mo)
Al6_FeMn	(6)(1)	(Al)(Fe,Mn)
Al8FeMnSi2	(16)(2)(2)(3)	(Al)(Fe)(Mn)(Si)
Bcc	(1)(3)	(Al,B,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti,Zr)(B,C,Va)
Cr3Mn5	(3)(5)	(Cr)(Mn)
Fcc	(1)(1)	(Al,B,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti,Zr)(B,C,Va)
FeMo3Si	(1)(3)(1)	(Fe)(Mo)(Si)
Hcp	(1)(0.5)	(Al,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti,Zr)(B,C,Va)
Laves_C14	(2)(1)	(Al,Cr,Fe,Hf,Mo,Ti,Zr)(Al,Cr,Fe,Hf,Mo,Ti,Zr)
Laves_C15	(2)(1)	(Al,Cr,Fe,Hf,Mo,Ti,Zr,Si)(Al,Cr,Fe,Hf,Mo,Ti,Zr)
Laves_C36	(2)(1)	(Cr,Zr)(Cr,Zr)
Liquid	(1)	(Al,B,C,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti,Zr)
Mn11Si19	(11)(19)	(Mn)(Si)
Mo3Al2C	(3)(2)(1)	(Mo)(Al)(C)
Mo3M3C	(3)(3)(1)	(Mo)(Fe,Mn)(C)
Mo4Si9Ti7	(0.55)(0.45)	(Mo,Ti)(Si)
Mo5Si3	(0.625)(0.375)	(Cr,Mo,Re,Si,Ti,Zr)(Al,B,Mo,Si)
Mo5Si3C	(4.8)(3)(0.6)	(Mo)(Si)(C)
Mo5SiB2	(0.625)(0.125)(0.25)	(Fe,Hf,Mn,Mo,Re,Ti,Zr)(B,Si)(B)
MoSi6Ti2	(1)(2)	(Mo,Ti)(Si)
MoSiZr	(1)(1)(1)	(Mo)(Si)(Hf,Mo,Zr)

1.4 Key Elements and Subsystems

The modeling status for the constituent binaries and ternaries of all the elements are given in Table 1.3 ~ Table 1.4. The color represents the following meaning:

: Full description

: Full description for major phases

: Extrapolation

Table 1.3: Modeling status for all the constituent binary systems

	B	C	Cr	Fe	Hf	Mn	Mo	Re	Si	Ti	Zr
Al											
B											
C											
Cr											
Fe											
Hf											
Mn											
Mo											
Re											
Si											
Ti											

Table 1.4: Modeling status for all the constituent ternary systems

Al-C-Mo	Al-Cr-Mo	Al-Fe-Mn	Al-Fe-Si	Al-Mn-Si	B-C-Mo	B-Hf-Mo	B-Mo-Re
B-Mo-Si	B-Mo-Zr	B-Si-Ti	C-Cr-Mo	C-Fe-Mo	C-Hf-Mo	C-Mn-Mo	C-Mo-Re
C-Mo-Si	C-Mo-Ti	C-Mo-Zr	Cr-Fe-Ti	Cr-Mo-Ti	Cr-Mo-Zr	Fe-Mo-Si	Hf-Mo-Si
Mo-Re-Si	Mo-Si-Ti	Mo-Si-Zr					

1.5 Database Validation

The current PanMo database was validated by large amounts of phase equilibrium data available for Mo alloys. A few examples are given here. Figure 1.1 shows the calculated liquidus projection of the Mo-Si-B ternary system. The calculated isothermal lines are also shown in the same figure.

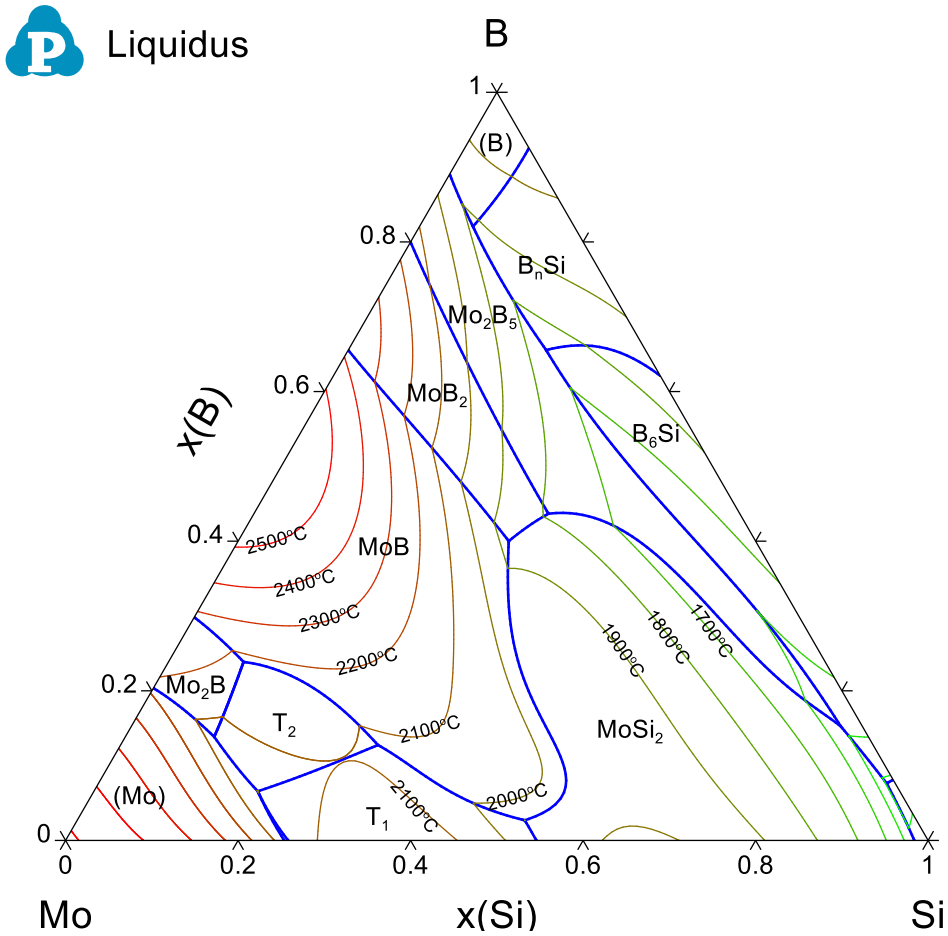


Figure 1.1: Calculated liquidus projection of the Mo-Si-B ternary system superimposed with the isothermal lines.

Figure 1.2 shows the calculated isothermal section of the Mo-Si-B ternary system at 1600°C, which demonstrates the equilibrium between the ternary T_2 phase and the binary phases.

Figure 1.3 and Figure 1.4 show the calculated isothermal sections of the Mo-Si-Ti ternary system with the experimental data of [2003Yan] at 1600°C and 1425°C, respectively. Blue lines are the calculated phase boundaries. Symbols are the phase equilibrium data measured using EPMA. It can be seen that the experimentally measured phase equilibrium data are in good agreement with the thermodynamic calculations using PanMo thermodynamic database.

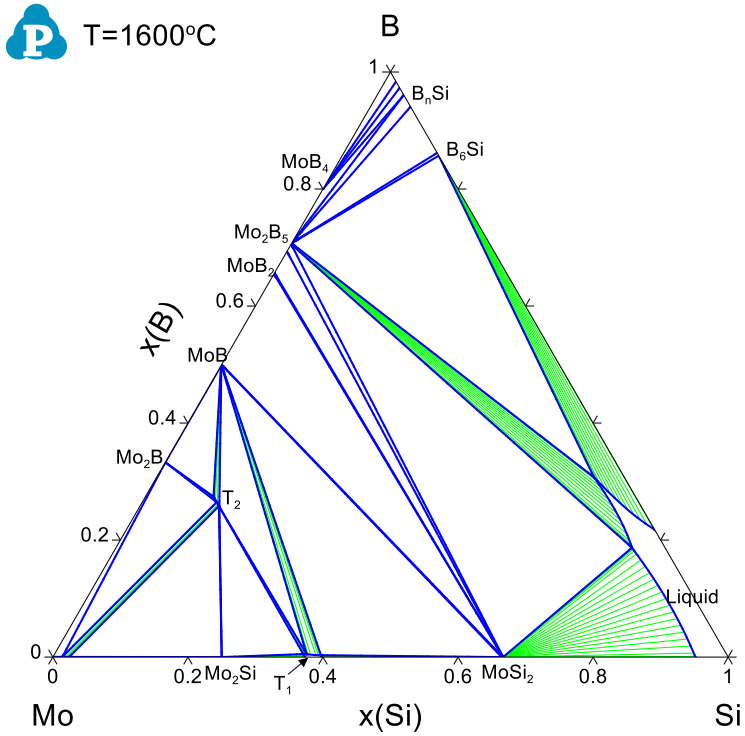


Figure 1.2: Calculated isothermal section of the Mo-Si-B ternary system at 1600°C

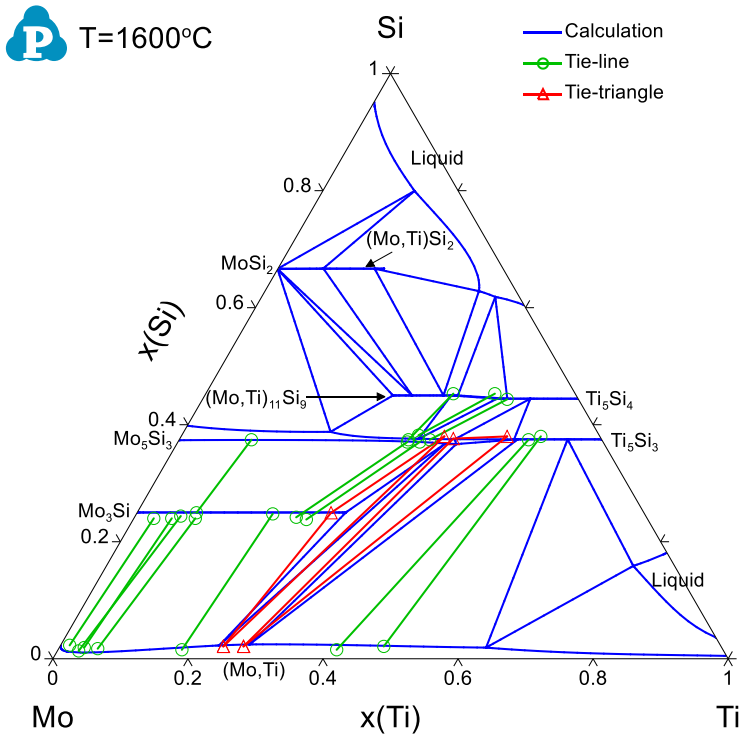


Figure 1.3: Calculated isothermal section of the Mo-Si-Ti ternary system at 1600°C with experimental data of [2003Yan] plotted on it

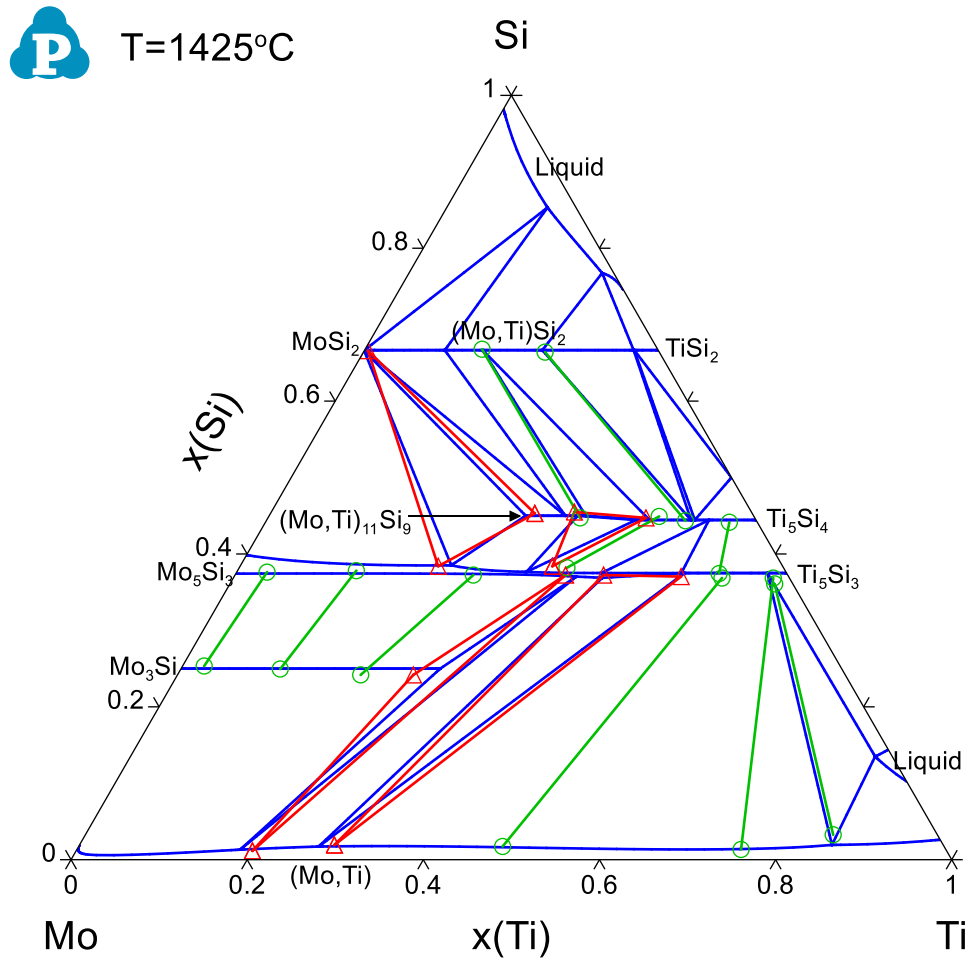
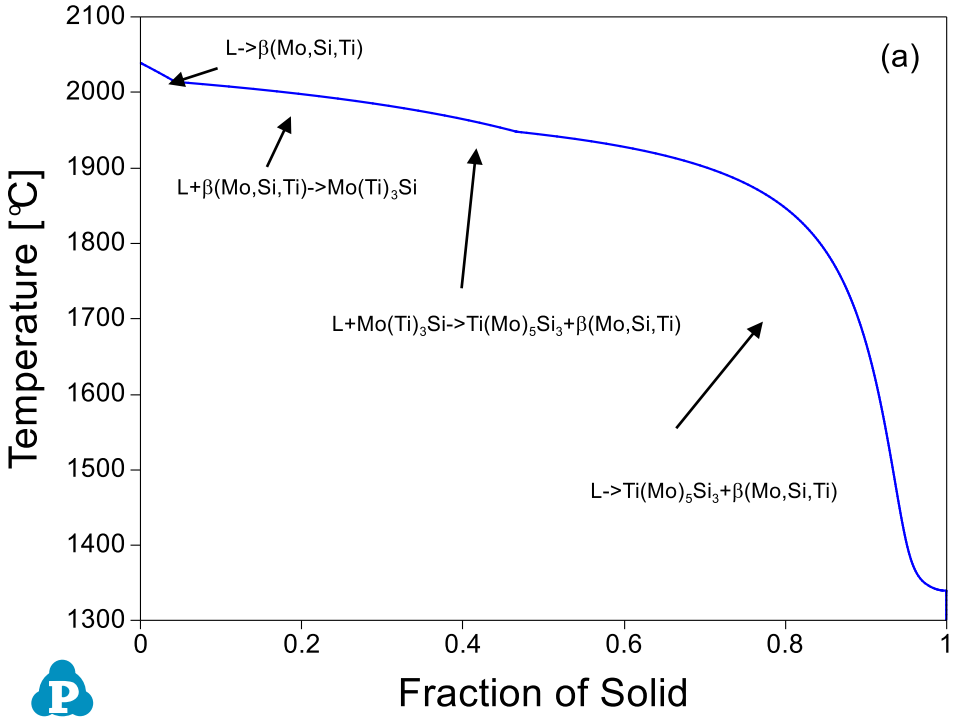
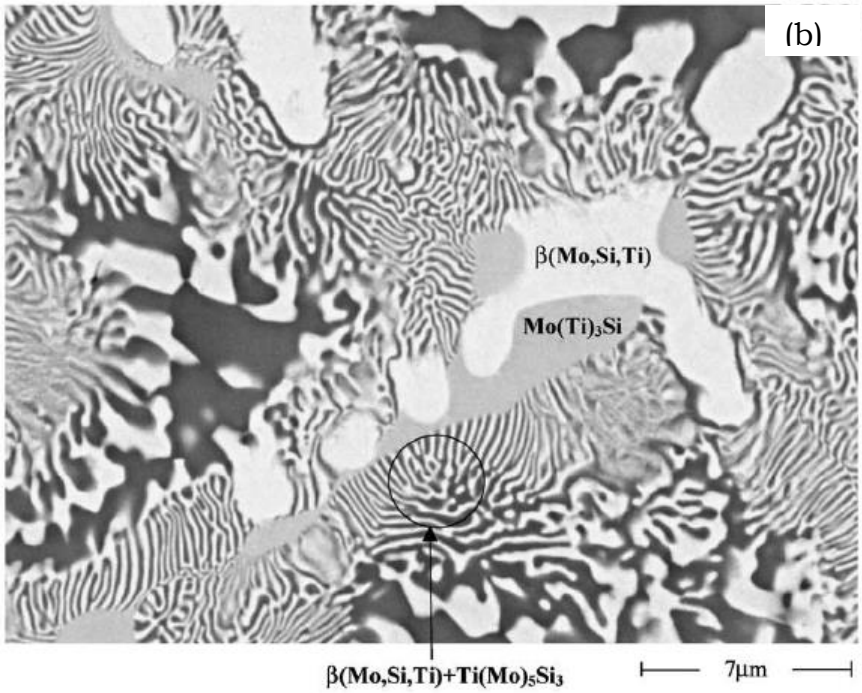
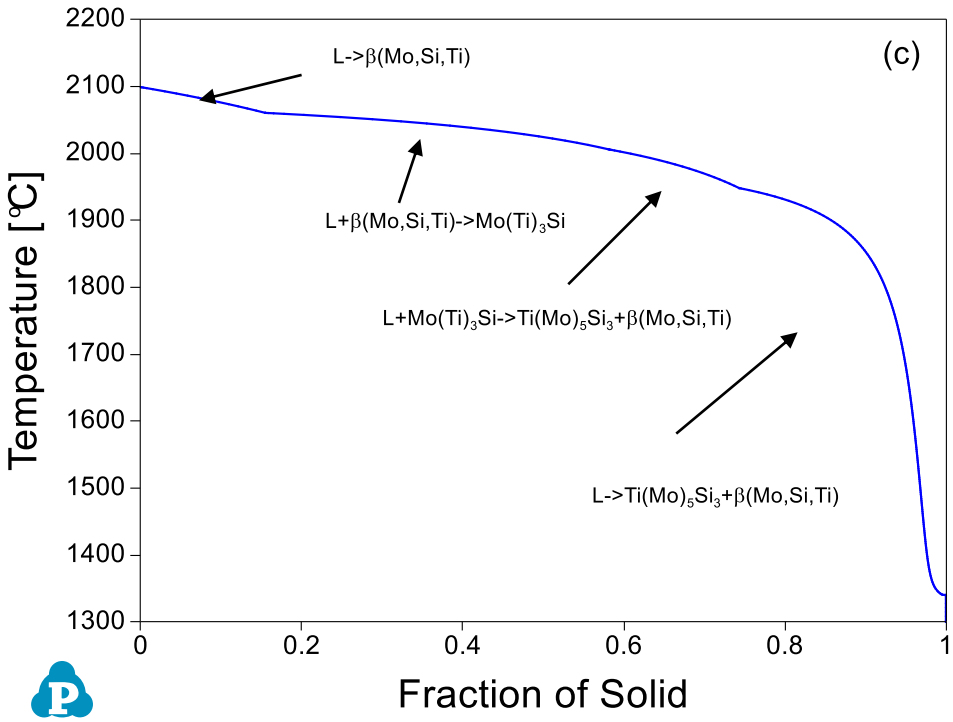


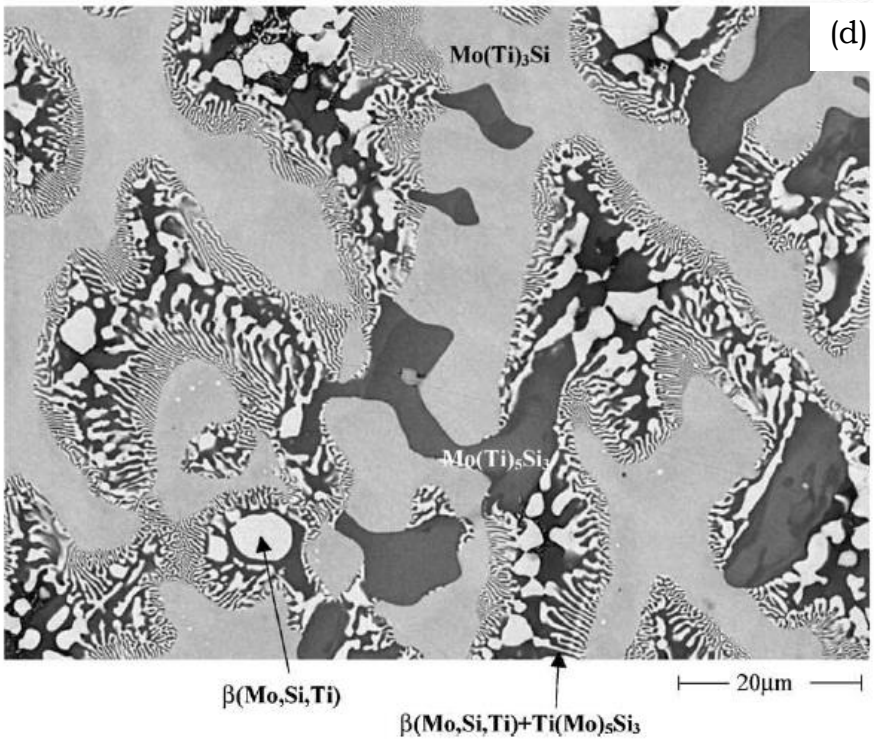
Figure 1.4: Calculated isothermal section of the Mo-Si-Ti ternary system at 1425°C with experimental data of [2003Yan] plotted on it

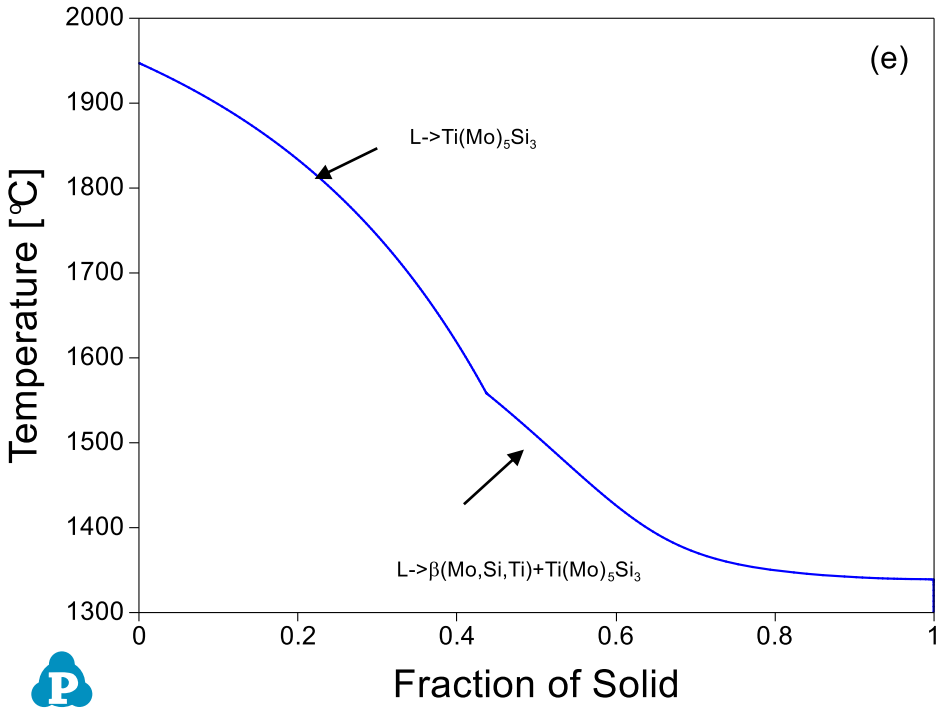
In addition to the validation of phase equilibria, the current database has also been subjected to extensive validation of solidification data of commercial aluminum alloys. Figure 1.5 presents the calculated fraction of solid vs. temperature of the Mo-Si-Ti alloys as well as the solidification sequence using the Scheil model. The back scattered images of the as-cast microstructure of these Mo-Si-Ti alloys from [2003Yan] are also shown in the same figure. The predicated microstructures of the Mo-Si-Ti alloys using the Scheil model agree well with experimental observations.


(a)
L->β(Mo,Si,Ti)
L+β(Mo,Si,Ti)->Mo(Ti)3Si
L+Mo(Ti)3Si->Ti(Mo)5Si3+β(Mo,Si,Ti)
L->Ti(Mo)5Si3+β(Mo,Si,Ti)
Temperature [℃]
Fraction of Solid
2100
2000
1900
1800
1700
1600
1500
1400
1300
0
0.2
0.4
0.6
0.8
1


(b)
β(Mo,Si,Ti)
Mo(Ti)3Si
β(Mo,Si,Ti)+Ti(Mo)5Si3
7μm


(c)
L->β(Mo,Si,Ti)
L+β(Mo,Si,Ti)->Mo(Ti)3Si
L+Mo(Ti)3Si->Ti(Mo)5Si3+β(Mo,Si,Ti)
L->Ti(Mo)5Si3+β(Mo,Si,Ti)
Temperature [°C]
Fraction of Solid
2200
2100
2000
1900
1800
1700
1600
1500
1400
1300
0
0.2
0.4
0.6
0.8
1


(d)
Mo(Ti)3Si
Mo(Ti)5Si3
β(Mo,Si,Ti)
β(Mo,Si,Ti)+Ti(Mo)5Si3
20μm



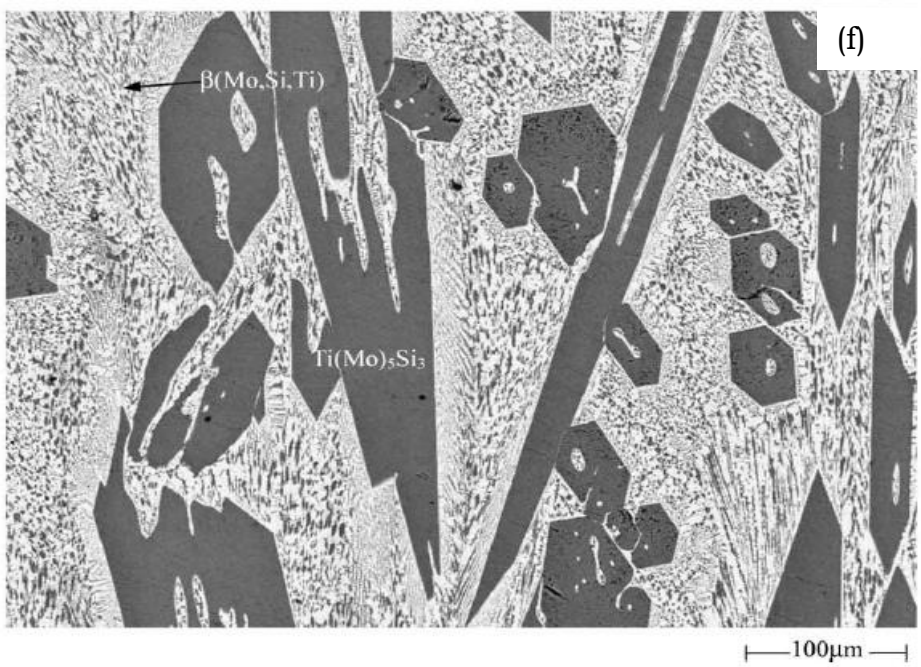


Figure 1.5: (a) Scheil simulation of solidification sequence of the $Mo_{40}Si_{20}Ti_{40}$ alloy; (b): BSE image of the as-cast microstructure of the $Mo_{40}Si_{20}Ti_{40}$ alloy; (c): Scheil simulation of the solidification sequence of the $Mo_{40}Si_{25}Ti_{35}$ alloy; (d): BSE image of the as-cast microstructure of the $Mo_{40}Si_{25}Ti_{35}$ alloy; (e): Scheil simulation of the solidification sequence of the $Mo_5Si_{25}Ti_{70}$ alloy; (f): BSE image of the as-cast microstructure of the $Mo_5Si_{25}Ti_{70}$ alloy

1.6 Reference

[2003Yan] Y. Yang, Y.A. Chang, L. Tan, Y. Du, Materials Science and Engineering A361 (2003) 281–293.