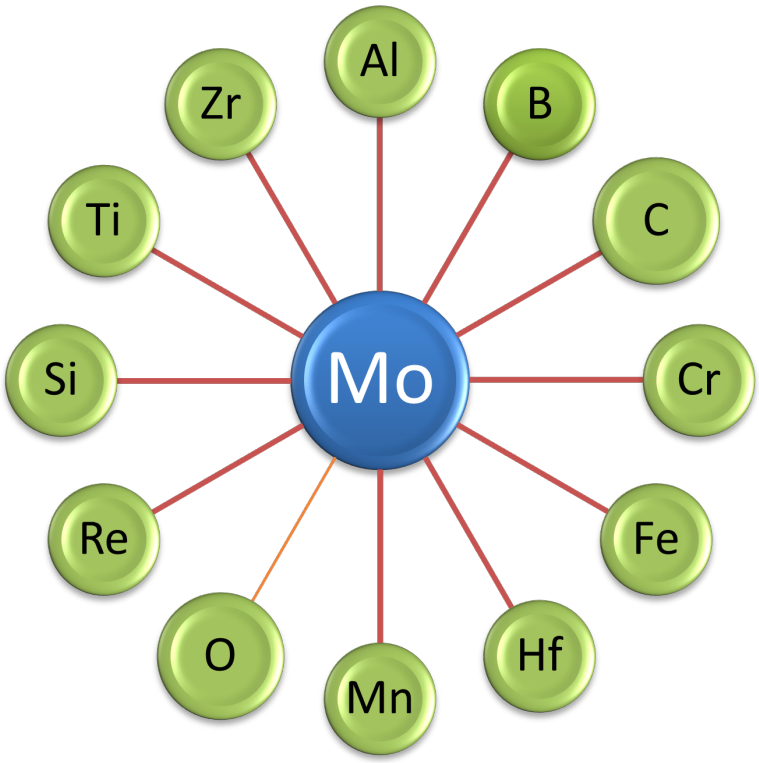
Pandat™ 2024

Database Manual

CompuTherm LLC

PanMolybdenum

Database for multi-component Molybdenum-rich alloys



PANDAT™
SOFTWARE

Contents

1 Thermodynamic Database

1.1 Components (13)

Total of **13** 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, O 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 1.5 .

Table 1.1: Suggested composition range

Elements	Composition Range (wt.%)
Mo	50 ~ 100
Si, Ti	0 ~ 30
B, Cr	0 ~ 20
Al, Hf, Mn, O, Re	0 ~ 10
C, Fe, Zr	0 ~ 5

1.3 What is new in PanMo2024

Addition of the component O.

1.4 Phases

Total of **208** phases are included in the database and a few key phases are listed in Table 1.2. Information on all the other phases is listed in PanMo2024:List of All Phases. Users can also view it through TDB viewer of Pandat™ .

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)
Bcc	(1)(3)	(Al,B,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti,Zr)(B,C,O,Va)
Fcc	(1)(1)	(Al,B,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti,Zr)(B,C,O,Va)
FeMo3Si	(1)(3)(1)	(Fe)(Mo)(Si)
Hcp	(1)(0.5)	(Al,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti,Zr)(B,C,O,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)
Liquid	(1)	(Al,B,C,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti,Zr,O,Al2O3, B2O3,Cr2/3O,FeO,FeO3/2,HfO2,MnO,Mn2/3O, MoO2,MoO3,SiO2,TiO,TiO3/2,TiO2,Zr1/2O)

Name	Lattice Size	Constituent
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)

1.5 Assessed Subsystems

A total of **88** subsystems, including 61 binary and 27 ternary subsystems have been assessed. The modeling status is indicated by numbers. The systems with number 10 are fully assessed in the whole composition range. The higher value shows higher reliability of the system.

Binary Systems (61)

Al-B(10)	Al-C(10)	Al-Cr(10)	Al-Fe(10)	Al-Hf(10)	Al-Mn(10)	Al-Mo(10)
Al-O(10)	Al-Re(10)	Al-Si(10)	Al-Ti(10)	Al-Zr(10)	B-Cr(10)	B-Fe(10)
B-Hf(10)	B-Mn(10)	B-Mo(10)	B-O(10)	B-Re(10)	B-Si(10)	B-Ti(10)
B-Zr(10)	Cr-Fe(10)	Cr-Hf(10)	Cr-Mn(10)	Cr-Mo(10)	Cr-O(10)	Cr-Re(10)

Cr-Si(10)	Cr-Ti(10)	Cr-Zr(10)	Fe-Hf(10)	Fe-Mn(10)	Fe-Mo(10)	Fe-O(10)
Fe-Re(10)	Fe-Si(10)	Fe-Ti(10)	Fe-Zr(10)	Hf-Mn(10)	Hf-Mo(10)	Hf-O(10)
Hf-Si(10)	Hf-Ti(10)	Hf-Zr(10)	Mn-Mo(10)	Mn-O(10)	Mn-Si(10)	Mo-O(10)
Mo-Re(10)	Mo-Si(10)	Mo-Ti(10)	Mo-Zr(10)	O-Re(5)	O-Si(10)	O-Ti(10)
Re-Si(10)	Re-Ti(10)	Si-Ti(10)	Si-Zr(10)	Ti-Zr(10)		

Ternary Systems (27)

Al-C-Mo(10)	Al-Cr-Mo(8)	Al-Fe-Mn(6)	Al-Fe-Si(10)	Al-Mn-Si(10)	B-C-Mo(10)
B-Hf-Mo(10)	B-Mo-Re(10)	B-Mo-Si(10)	B-Mo-Zr(5)	B-Si-Ti(10)	C-Cr-Mo(10)
C-Fe-Mo(10)	C-Hf-Mo(10)	C-Mn-Mo(10)	C-Mo-Re(10)	C-Mo-Si(10)	C-Mo-Ti(10)
C-Mo-Zr(10)	Cr-Fe-Ti(10)	Cr-Mo-Ti(10)	Cr-Mo-Zr(10)	Fe-Mo-Si(10)	Hf-Mo-Si(10)
Mo-Re-Si(10)	Mo-Si-Ti(10)	Mo-Si-Zr(8)			

1.6 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.

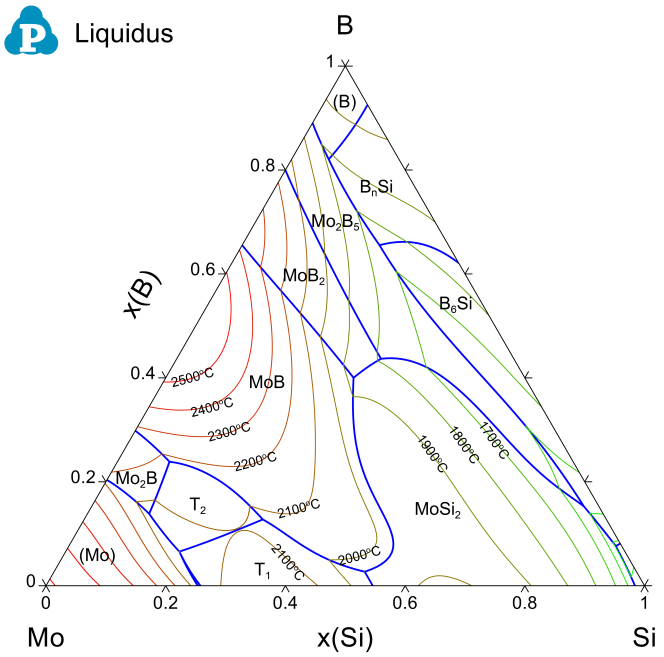


Figure 1.1: Calculated liquidus projection of the Mo-Si-B ternary system superimposed with the isothermal lines.

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.

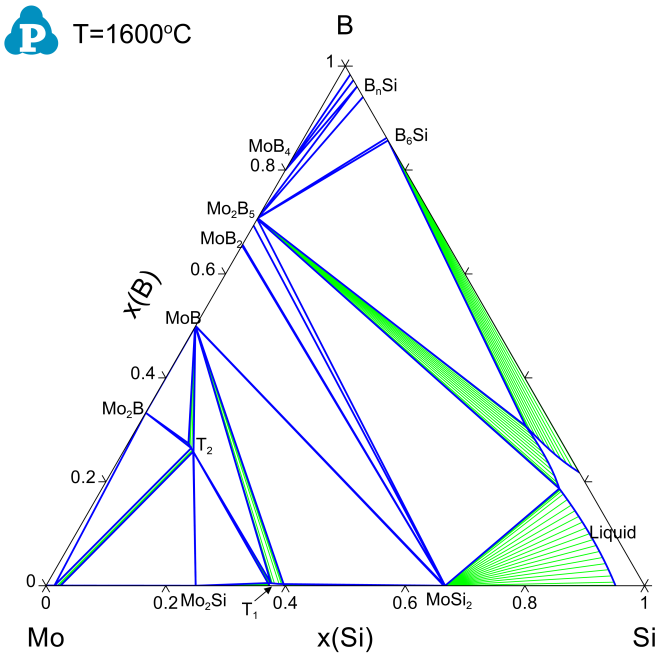


Figure 1.2: Calculated isothermal section of the Mo-Si-B ternary system at 1600 °C

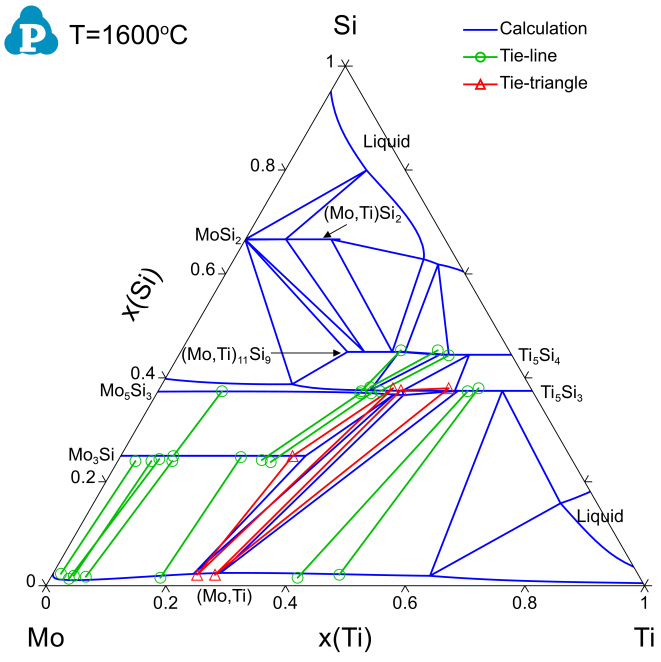


Figure 1.3: Calculated isothermal section of the Mo-Si-Ti ternary system at 1600 °C with experimental data of [2003Yan] plotted on it

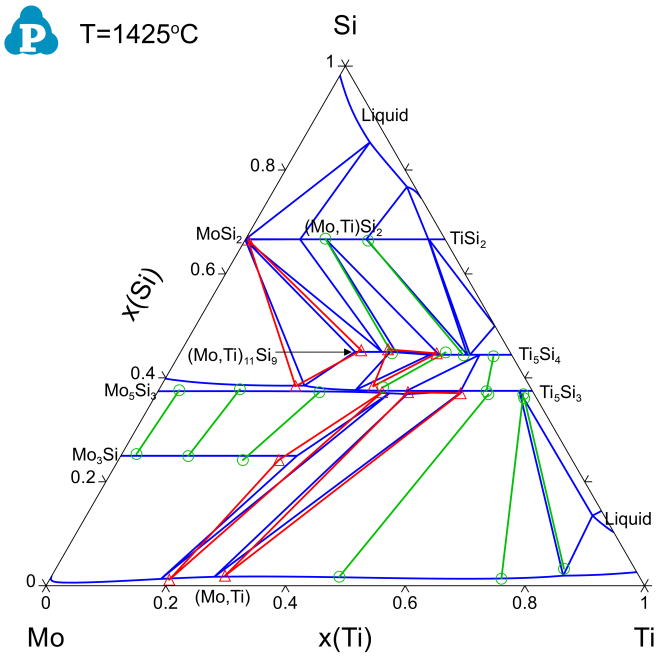
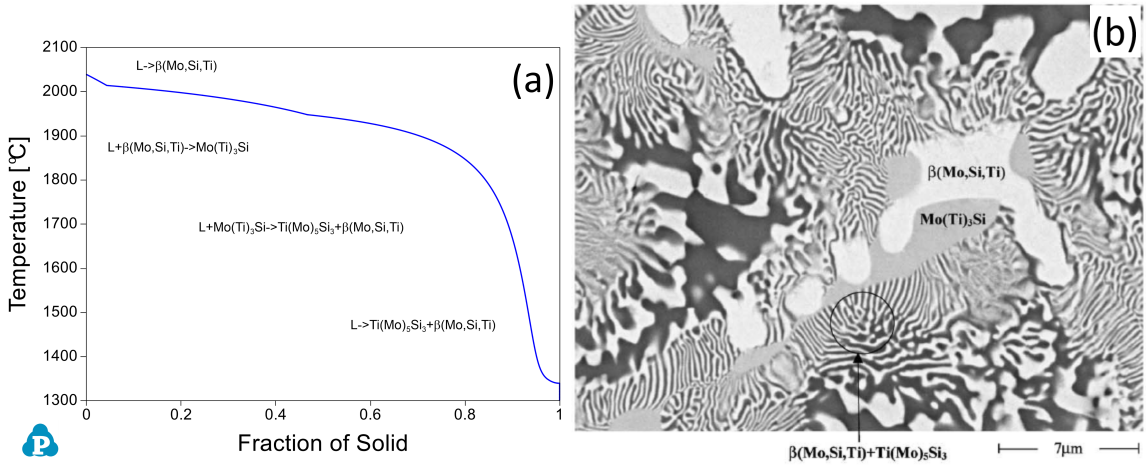


Figure 1.4: Calculated isothermal section of the Mo-Si-Ti ternary system at 1425 °C with experimental data of [2003Yan] plotted on it

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.



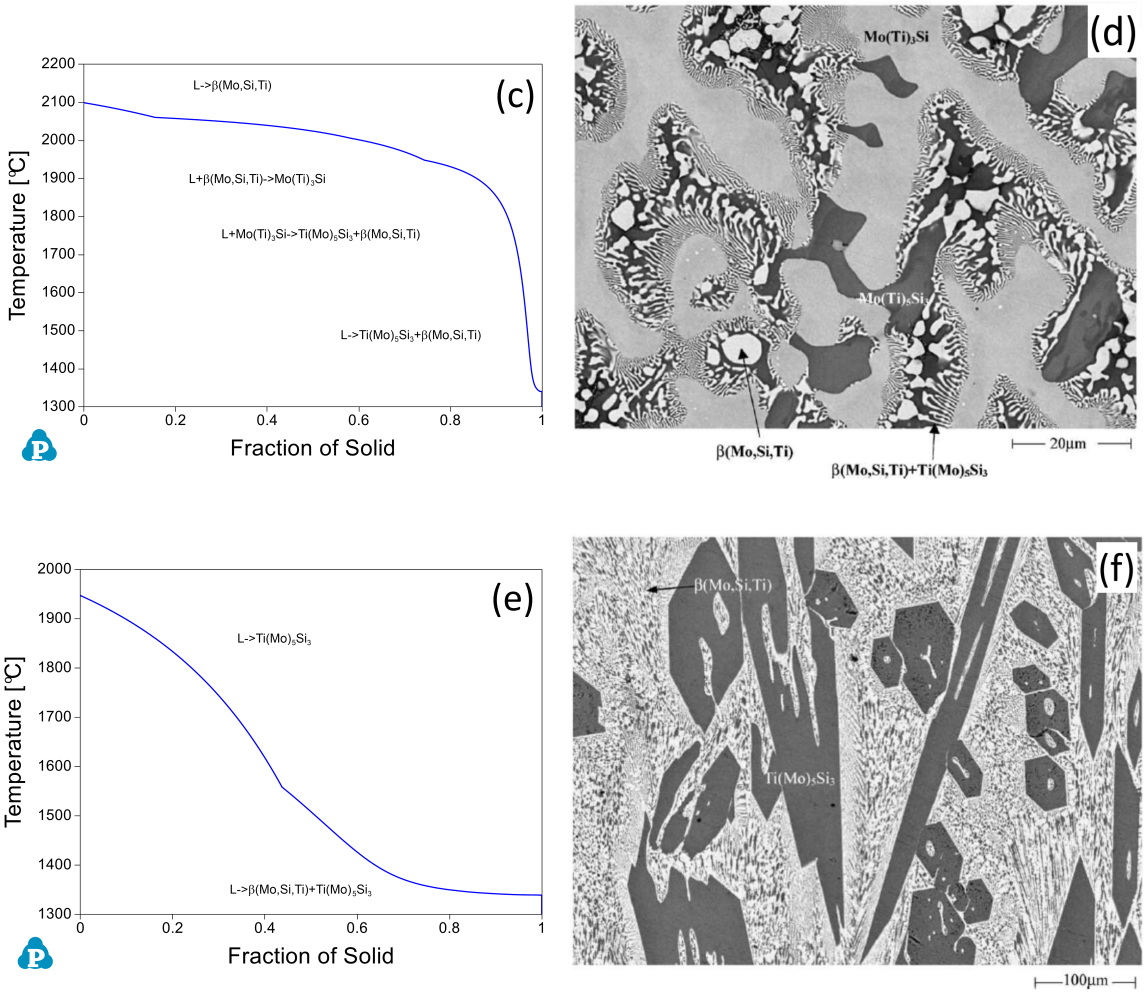


Figure 1.5: (a) Scheil simulation of solidification sequence of the Mo40Si20Ti40 alloy; (b): BSE image of the as-cast microstructure of the Mo40Si20Ti40 alloy; (c): Scheil simulation of the solidification sequence of the Mo40Si25Ti35 alloy; (d): BSE image of the as-cast microstructure of the Mo40Si25Ti35 alloy; (e): Scheil simulation of the solidification sequence of the Mo5Si25Ti70 alloy; (f): BSE image of the as-cast microstructure of the Mo5Si25Ti70 alloy

2 Mobility Database

PanMo2024_MB is an atomic mobility database for Mo-based alloys, which is compatible with the `PanMo2024_TH` thermodynamic database and suitable for the simulation of diffusion-controlled phenomena using the **PanDiffusion** module, **PanEvolution** module, and/or **PanSolidification** module.

2.1 Phases

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

2.2 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	Cr	Fe	Hf	Mn	Mo	Re	Si	Ti	Zr
Bcc										
Fcc										
Hcp										

2.3 Assessed Systems

In addition to the assessed self-diffusivities shown above, the impurity diffusion data for all elements included in the current `PanMo2024_MB` mobility database are also assessed. Moreover, chemical-diffusivities available in some binary and ternary systems are also used to assess the interaction parameters. These binary and ternary systems are listed below for the Bcc, Fcc, and Hcp phases, respectively.

Fcc Phase

Al-Si	Cr-Fe	Fe-Si	Fe-Mn	Fe-Mn-Si

Bcc phase

Al-Fe	Al-Ti	Cr-Fe	Cr-Ti	Fe-Ti	Hf-Zr	Mo-Zr

2.4 Database Validation

The simulated concentration profiles of a series of Mo-based alloys are shown below to validate the current `PanMo2024_MB` database.

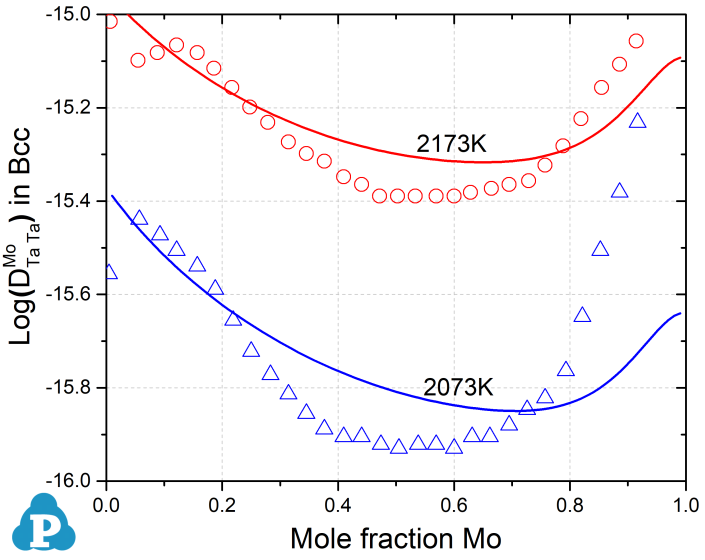


Figure 2.1: Inter-diffusion coefficients of Ta in bcc Mo-Ta binary alloys [2012Liu]

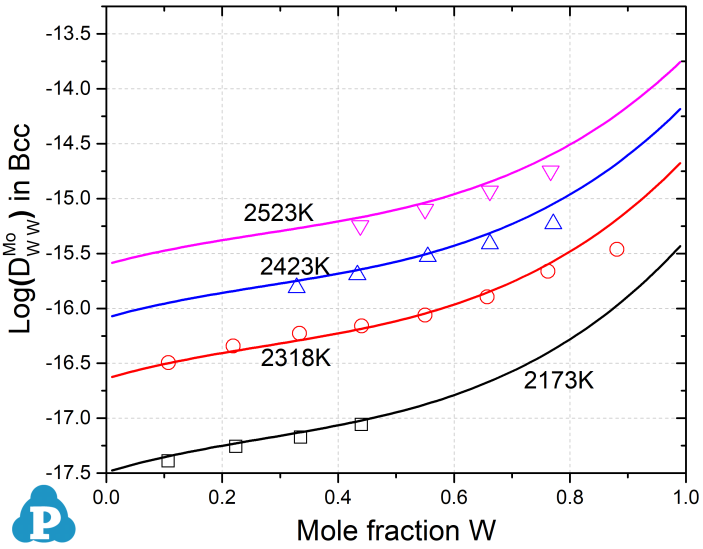


Figure 2.2: Inter-diffusion coefficients of W in bcc Mo-W binary alloys [2012Liu]

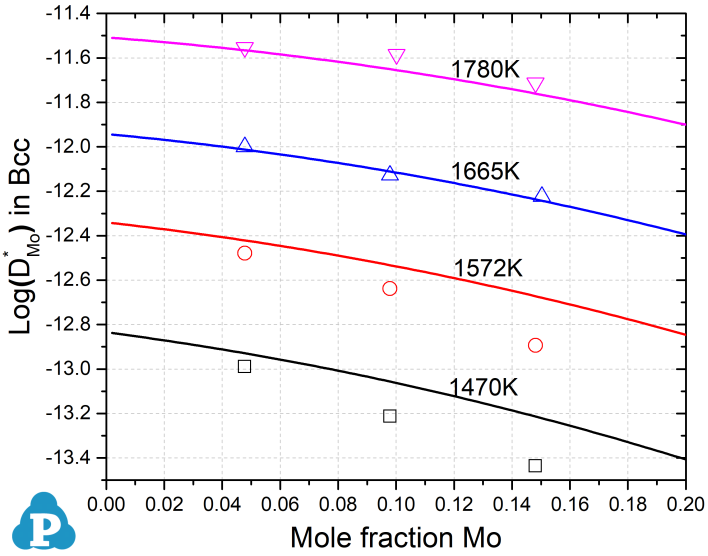


Figure 2.3: Tracer diffusion of Mo in bcc Mo-Zr alloys at different temperatures [2013Liu]

3 Thermophysical Property Database

The thermophysical property database **PanMo2024_TP**is compatible with the `PanMo2024_TH` thermodynamic database and suitable for the simulation of thermophysical properties of Mo-based alloys. It includes the molar volume data for all the phases, surface tension and viscosity properties for the liquid phase.

3.1 Molar Volume

The current molar volume database covers all **208** phases assessed in the `PanMo2024_TH` database. It is used to calculate the density, thermal expansion, solidification shrinkage of Mo alloys.

The simulated density changes vs. temperature of a series of Mo-based alloys are shown below to validate the current `PanMo2024_MV` database.

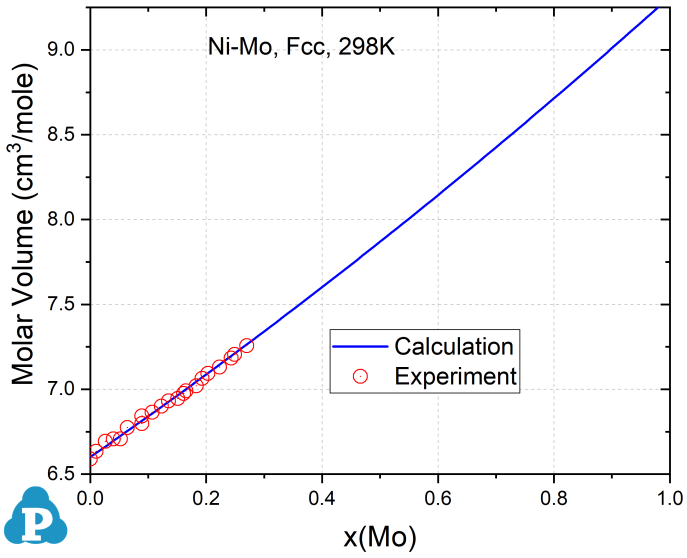


Figure 3.1: Molar volume of Ni-Mo Fcc binary alloys at 298K [2004Fan, 2014Li]

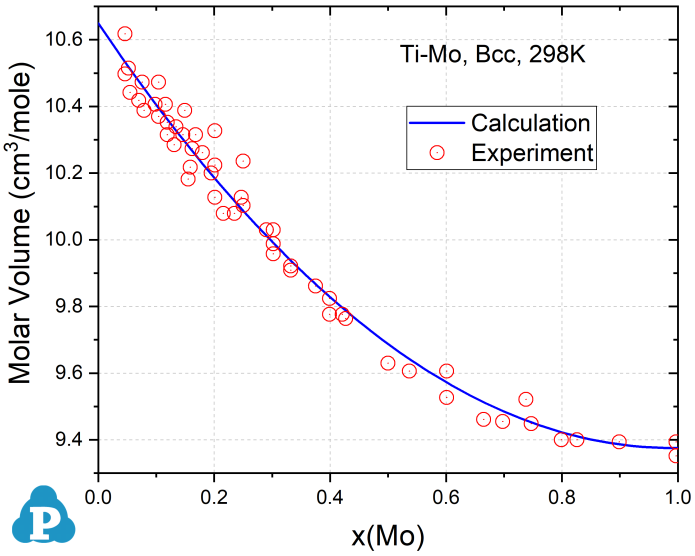


Figure 3.2: Molar volume of Ti-Mo Bcc binary alloys at 298K [2016Yan]

4 References

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

[2004Fan] L. Fang, Density of Liquid Ni-Mo Alloys Measured by a Modified Sessile Drop Method. Journal of materials science & technology, 2004. 20(3): p. 287-292.

[2012Liu] Y. Liu, et al., Diffusion characteristics and atomic mobilities for bcc refractory Mo-Ta, Mo-W, and Mo-Nb alloys. Calphad, 2012. 36: p. 110-117.

[2013Liu] Y. Liu, et al., Mobilities and diffusivities for bcc Nb-W, Nb-Ta, Zr-Mo and Zr-Hf alloys. Journal of Alloys and Compounds, 2013. 555: p. 381-389.

[2014Li] J. Li, X.-G. Lu and Y. He, Molar Volume of Fcc Phase in the Ni-Cr-Mo System. Advanced Materials Research, 2014. 936: p. 1209-1215.

[2016Yan] J.-Y. Yan and G.B. Olson, Molar volumes of bcc, hcp, and orthorhombic Ti-base solid solutions at room temperature. Calphad, 2016. 52: p. 152-158.

PanMo2024:List of All Phases

Phases (**208**)

Name	Model	Lattice Size	Constituent
ABMo	CEF (SLN)	(0.5)(0.5)	(Cr,Mo,Ti)(B,Va)
ALPHA_ RHOMBO_B	CEF (ST1)	(1)	(B)
A_TiO	CEF (ST2)	(1)(1)	(Ti)(O)
Al11Cr2	CEF (ST2)	(10)(1)(2)	(Al)(Al)(Cr)
Al11Mn4	CEF (SLN)	(11)(4)	(Al)(Fe,Mn)
Al11Mn4_HT	CEF (SLN)	(29)(10)	(Al,Mn)(Mn)
Al11Re4	CEF (ST2)	(11)(4)	(Al)(Re)
Al12Mn	CEF (SLN)	(12)(1)	(Al)(Fe,Mn)
Al12Mo	CEF (ST2)	(0.923)(0.077)	(Al)(Mo)
Al12Re	CEF (ST2)	(12)(1)	(Al)(Re)
Al13Cr2	CEF (ST2)	(13)(2)	(Al)(Cr)
Al13Fe4	CEF (SLN)	(0.6275) (0.235) (0.1375)	(Al)(Fe,Mn)(Al,Si,Va)
Al15_ FeMn3Si2	CEF (SLN)	(16)(4)(1)(2)	(Al)(Fe,Mn)(Si)(Al,Si)
Al1Fe1O3	CEF (ST3)	(1)(1)(3)	(Al+3)(Fe+3)(O-2)
Al2Fe	CEF (SLN)	(2)(1)	(Al)(Fe,Mn)
Al2Hf	CEF (ST2)	(0.666667) (0.333333)	(Al)(Hf)

Name	Model	Lattice Size	Constituent
Al2Hf3	CEF (ST2)	(0.4)(0.6)	(Al)(Hf)
Al2Ti	CEF (ST2)	(2)(1)	(Al)(Ti)
Al2Zr	CEF (SLN)	(0.666667) (0.333333)	(Al,Mo)(Zr)
Al2Zr3	CEF (ST2)	(0.4)(0.6)	(Al)(Zr)
Al3Hf	CEF (ST2)	(0.75)(0.25)	(Al)(Hf)
Al3Hf2	CEF (ST2)	(0.6)(0.4)	(Al)(Hf)
Al3Hf4	CEF (ST2)	(0.428571) (0.571429)	(Al)(Hf)
Al3Ti	CEF (SLN)	(0.25)(0.75)	(Al,Ti)(Al,Ti)
Al3Zr	CEF (ST2)	(0.75)(0.25)	(Al)(Zr)
Al3Zr2	CEF (ST2)	(0.6)(0.4)	(Al)(Zr)
Al3Zr4	CEF (ST2)	(0.42857) (0.57143)	(Al)(Zr)
Al3Zr5	CEF (ST2)	(0.375)(0.625)	(Al)(Zr)
Al4C3	CEF (SLN)	(4)(3)	(Al,Mo,Si)(C)
Al4Cr	CEF (ST2)	(4)(1)	(Al)(Cr)
Al4Mn	CEF (SLN)	(4)(1)	(Al)(Fe,Mn)
Al4Mn_L	CEF (ST2)	(461)(107)	(Al)(Mn)
Al4Mo	CEF (SLN)	(0.8)(0.2)	(Al,Fe)(Mo)
Al4Mo3Ti3	CEF (ST3)	(4)(3)(3)	(Al)(Mo)(Ti)
Al4Re	CEF (ST2)	(4)(1)	(Al)(Re)
Al4Zr5	CEF (ST2)	(0.444444) (0.555556)	(Al)(Zr)
Al5Fe2	CEF (SLN)	(5)(2)	(Al)(Fe,Mn)
Al5Fe4	CEF (SLN)	(1)	(Al,Fe,Mn)

Name	Model	Lattice Size	Constituent
Al5Mo	CEF (ST2)	(0.833)(0.167)	(Al)(Mo)
Al5Ti2	CEF (ST2)	(5)(2)	(Al)(Ti)
Al63Mo37	CEF (ST2)	(0.63)(0.37)	(Al)(Mo)
Al6Re	CEF (ST2)	(6)(1)	(Al)(Re)
Al6_FeMn	CEF (SLN)	(6)(1)	(Al)(Fe,Mn)
Al8Cr5_H	CEF (ST2)	(8)(5)	(Al)(Cr)
Al8Cr5_L	CEF (ST2)	(8)(5)	(Al)(Cr)
Al8FeMnSi2	CEF (ST4)	(16)(2)(2)(3)	(Al)(Fe)(Mn)(Si)
Al8FeMo3	CEF (SLN)	(8)(1)(3)	(Al)(Al,Fe)(Mo)
Al8Mn5	CEF (SLN)	(12)(5)(9)	(Al)(Mn)(Al,Mn)
Al8Mo3	CEF (ST2)	(0.727)(0.273)	(Al)(Mo)
Al9Cr4_H	CEF (ST2)	(9)(4)	(Al)(Cr)
Al9Cr4_L	CEF (ST2)	(9)(4)	(Al)(Cr)
AlB12_Alpha	CEF (ST2)	(1)(12)	(Al)(B)
AlCr2	CEF (ST2)	(1)(2)	(Al)(Cr)
AlHf	CEF (ST2)	(0.5)(0.5)	(Al)(Hf)
AlHf2	CEF (ST2)	(0.333333) (0.666667)	(Al)(Hf)
AlMnSi_Beta	CEF (SLN)	(15)(1)(4)(6)	(Al)(Si)(Al,Si)(Mn)
AlMoSi_C54	CEF (ST3)	(0.434)(0.333) (0.233)	(Al)(Mo)(Si)
AlRe	CEF (ST2)	(1)(1)	(Al)(Re)
AlRe2	CEF (ST2)	(1)(2)	(Al)(Re)
AlTi	CEF (SLN)	(0.5)(0.5)	(Al,Ti)(Al,Ti)
AlTi3	CEF (SLN)	(0.75)(0.25)	(Al,Ti)(Al,Ti)

Name	Model	Lattice Size	Constituent
AlZr	CEF (ST2)	(0.5)(0.5)	(Al)(Zr)
AlZr2	CEF (ST2)	(0.333333) (0.666667)	(Al)(Zr)
AlZr3	CEF (ST2)	(0.25)(0.75)	(Al)(Zr)
Alpha-Mn2B	CEF (ST2)	(0.670691) (0.329309)	(Mn)(B)
Alpha_AlFeSi	CEF (SLN)	(0.66)(0.19) (0.05)(0.1)	(Al)(Fe)(Si)(Al,Si)
B2	CEF (SLN)	(1)(1)	(Al,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti) (Al,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti,Va)
B2O3	CEF (ST2)	(2)(3)	(B)(O)
B3Si	CEF (SLN)	(6)(2)(6)	(B)(Si)(B,Si)
B4C	CEF (SLN)	(1)(1)	(B12,B11C)(B2,B2C,BC2)
B4Mo	CEF (ST2)	(0.8)(0.2)	(B)(Mo)
B5Mo2	CEF (SLN)	(2)(5)	(Mo)(B,Va)
B6Si	CEF (SLN)	(210)(23)(48)	(B)(Si)(B,Si)
BETA_ RHOMBO_B	CEF (SLN)	(93)(12)	(B,Re)(B,Mn,Si,Zr)
BMo	CEF (SLN)	(0.5)(0.5)	(B)(Mo,Ti)
B_NSi	CEF (SLN)	(61)(1)(8)	(B)(Si)(B,Si)
Bcc	CEF (SLN)	(1)(3)	(Al,B,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti,Zr) (B,C,O,Va)
Bcc_B2	CEF (SLN)	(0.5)(0.5)(3)	(Al,Fe,Si)(Al,Fe,Si)(Va)
Beta_AlFeSi	CEF (SLN)	(0.598)(0.152) (0.1)(0.15)	(Al)(Fe,Mn)(Si)(Al,Si)
CBCC_A12	CEF (SLN)	(1)(1)	(Al,Cr,Fe,Mn,Mo,Re,Si,Ti,Zr)(C,Va)

Name	Model	Lattice Size	Constituent
CUB_A13	CEF (SLN)	(1)(1)	(Al,Cr,Fe,Hf,Mn,Mo,Si,Ti,Zr)(C,Va)
Cementite	CEF (SLN)	(3)(1)	(Cr,Fe,Mo)(C)
Chi_A12	CEF (SLN)	(24)(10)(24)	(Cr,Fe,Re)(Cr,Mo,Re)(Cr,Fe,Mo,Re)
Corundum	CEF (SLN)	(2)(1)(3)	(Al+3,Cr+2,Cr+3,Fe+2,Fe+3,Ti+3,Va) (Cr+3,Fe+3,Va)(O-2)
Cr3B4	CEF (ST2)	(0.429)(0.571)	(Cr)(B)
Cr3Mn5	CEF (ST2)	(3)(5)	(Cr)(Mn)
Cr5B3	CEF (ST2)	(0.625)(0.375)	(Cr)(B)
CrB	CEF (ST2)	(0.5)(0.5)	(Cr)(B)
CrB2	CEF (SLN)	(0.333)(0.667)	(Cr)(B,Va)
CrB4	CEF (ST2)	(0.2)(0.8)	(Cr)(B)
CrSi	CEF (ST2)	(0.5)(0.5)	(Cr)(Si)
CrSi2	CEF (ST2)	(1)(2)	(Cr)(Si)
Cristobalite	CEF (ST2)	(1)(2)	(Si)(O)
DISORDER	CEF (SLN)	(1)	(Al,Cr)
Delta	CEF (SLN)	(3)(1)	(Al,Cr,Fe,Mo,Re,Ti)(Al,Cr,Fe,Hf,Mo,Ti)
Diamond	CEF (SLN)	(1)	(Al,B,C,Si,Ti)
Eta	CEF (SLN)	(0.75)(0.25)	(Fe,Ti)(Al,Cr,Hf,Mo,Ti)
Fcc	CEF (SLN)	(1)(1)	(Al,B,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti,Zr) (B,C,O,Va)
Fe23Zr6	CEF (ST2)	(0.793)(0.207)	(Fe)(Zr)
Fe2Si	CEF (ST2)	(0.666667) (0.333333)	(Fe)(Si)
Fe4Re	CEF (SLN)	(4)(1)	(Fe,Re)(Fe,Re)
Fe5Si3	CEF (ST2)	(0.625)(0.375)	(Fe)(Si)
FeHf2	CEF (ST2)	(0.3333)	(Fe)(Hf)

Name	Model	Lattice Size	Constituent
		(0.6667)	
FeMo3Si	CEF (ST3)	(1)(3)(1)	(Fe)(Mo)(Si)
FeSi	CEF (ST2)	(0.5)(0.5)	(Fe)(Si)
FeSi2_H	CEF (ST2)	(3)(7)	(Fe)(Si)
FeSi2_L	CEF (ST2)	(1)(2)	(Fe)(Si)
FeZr2	CEF (SLN)	(1)(2)	(Fe,Zr)(Fe,Zr)
FeZr3	CEF (SLN)	(1)(3)	(Fe,Zr)(Fe,Zr)
GAS	GAS	(1)	(B,B2,Mn,Mo,MO2,Re,Si,Si2,Si3,Al, AlO,AlO2,Al2,Al2O,Al2O2,Al2O3, C1O1,C1O2,Fe,FeO,FeO2,Fe2,Hf, HfO,HfO2,O,O2,O3,SiO,SiO2, Ti,TiO,TiO2,Zr,Zr2,ZrO,ZrO2)
Gamma_ AlFeSi	CEF (ST3)	(0.635)(0.205) (0.16)	(Al)(Fe)(Si)
Graphite	CEF (SLN)	(1)	(B,C)
H_Sigma	CEF (SLN)	(8)(4)(18)	(Mn)(Cr)(Cr,Mn)
Halite	CEF (SLN)	(1)(1)	(Al+3,Cr+3,Fe+2,Fe+3,Mn+2,Mn+3,Va) (O-2,Va)
Hcp	CEF (SLN)	(1)(0.5)	(Al,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti,Zr) (B,C,O,Va)
HfMn	CEF (ST2)	(0.5)(0.5)	(Hf)(Mn)
HfMn2	CEF (SLN)	(1)(2)	(Hf,Mn)(Hf,Mn)
HfSiO4	CEF (ST3)	(1)(1)(4)	(Hf)(Si)(O)
L10_FCC	CEF (SLN)	(0.5)(0.5)	(Al,Ti)(Al,Ti)
L12_FCC	CEF (SLN)	(0.75)(0.25)	(Al,Cr)(Al,Cr)
Laves_C14	CEF (SLN)	(2)(1)	(Al,Cr,Fe,Hf,Mo,Ti,Zr)

Name	Model	Lattice Size	Constituent
			(Al,Cr,Fe,Hf,Mo,Ti,Zr)
Laves_C15	CEF (SLN)	(2)(1)	(Al,Cr,Fe,Hf,Mo,Ti,Zr,Si) (Al,Cr,Fe,Hf,Mo,Ti,Zr)
Laves_C36	CEF (SLN)	(2)(1)	(Cr,Zr)(Cr,Zr)
Liquid	CEF (SLN)	(1)	(Al,B,C,Cr,Fe,Hf,Mn,Mo,Re,Si,Ti, Zr,O,Al2O3,B2O3,Cr2/3O,FeO, FeO3/2,HfO2,MnO,Mn2/3O, MoO2,MoO3,SiO2,TiO,TiO3/2, TiO2,Zr1/2O)
M23C6	CEF (SLN)	(23)(6)	(Cr,Fe,Mn,Mo)(C)
M2B_Ti12	CEF (SLN)	(0.333)(0.667)	(B,Si)(Cr,Fe,Hf,Mn,Mo,Re,Ti,Zr)
M3B2	CEF (SLN)	(2)(3)	(B,Si)(Fe,Mn,Mo,Hf,Zr)
M3B4	CEF (SLN)	(4)(3)	(B)(Hf,Mn,Ti)
M3C2	CEF (SLN)	(3)(2)	(Cr,Mo)(C)
M7C3	CEF (SLN)	(7)(3)	(Cr,Fe,Mn,Mo,Re)(C)
MB2_HP3	CEF (SLN)	(1)(2)	(Al,Cr,Hf,Mn,Mo,Ti,Zr)(B,Va)
MB_OP8	CEF (SLN)	(1)(1)	(B,Si)(Fe,Hf,Mn,Mo,Ti,Zr)
MSi2_C11b	CEF (SLN)	(0.333)(0.667)	(Mo,Re)(Al,Si,Va)
MSi2_Ti6	CEF (SLN)	(1)(2)	(Mo,Re)(Al,Si,Va)
Mn11Si19	CEF (ST2)	(11)(19)	(Mn)(Si)
Mn3C	CEF (ST2)	(3)(1)	(Mn)(C)
Mn3O4_A	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3O4_B	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3Si	CEF (ST2)	(3)(1)	(Mn)(Si)
Mn5C2	CEF (ST2)	(5)(2)	(Mn)(C)
Mn6Si	CEF (ST2)	(17)(3)	(Mn)(Si)

Name	Model	Lattice Size	Constituent
Mn9Si2	CEF (ST2)	(33)(7)	(Mn)(Si)
MnB4	CEF (ST2)	(0.2)(0.8)	(Mn)(B)
Mo2BC	CEF (ST3)	(2)(1)(1)	(Mo)(B)(C)
Mo2Fe21C6	CEF (ST3)	(2)(21)(6)	(Mo)(Fe)(C)
Mo2Hf	CEF (SLN)	(2)(1)(1)	(Hf,Mo,Si)(Hf,Mo)(C,Va)
Mo2Mn4C	CEF (ST3)	(2)(4)(1)	(Mo)(Mn)(C)
Mo3Al2C	CEF (ST3)	(3)(2)(1)	(Mo)(Al)(C)
Mo3M3C	CEF (SLN)	(3)(3)(1)	(Mo)(Fe,Mn)(C)
Mo3Si	CEF (SLN)	(0.75)(0.25)	(Cr,Fe,Hf,Mo,Re,Si,Ti,Zr) (Al,Cr,Fe,Re,Si)
Mo4O11	CEF (ST2)	(0.266667) (0.733333)	(Mo)(O)
Mo4Si9Ti7	CEF (SLN)	(0.55)(0.45)	(Mo,Ti)(Si)
Mo5Si3	CEF (SLN)	(0.625)(0.375)	(Cr,Mo,Re,Si,Ti,Zr)(Al,B,Mo,Si)
Mo5Si3C	CEF (ST3)	(4.8)(3)(0.6)	(Mo)(Si)(C)
Mo5SiB2	CEF (SLN)	(0.625)(0.125) (0.25)	(Fe,Hf,Mn,Mo,Re,Ti,Zr)(B,Si)(B)
Mo8O23	CEF (ST2)	(0.258064) (0.741935)	(Mo)(O)
Mo9O26	CEF (ST2)	(0.257143) (0.742857)	(Mo)(O)
MoO3	CEF (ST2)	(1)(3)	(Mo)(O)
MoSi6Ti2	CEF (SLN)	(1)(2)	(Mo,Ti)(Si)
MoSiZr	CEF (SLN)	(1)(1)(1)	(Mo)(Si)(Hf,Mo,Zr)
Mu_Phase	CEF (SLN)	(7)(2)(4)	(Al,Cr,Fe,Mn,Mo,Re,Si)(Cr,Mo,Re,Ti) (Cr,Fe,Mo,Re,Ti)

Name	Model	Lattice Size	Constituent
P_PHASE	CEF (SLN)	(24)(12)(20)	(Cr,Fe,Re)(Mo)(Cr,Fe,Mo,Re)
Quartz	CEF (ST2)	(1)(2)	(Si)(O)
R_Phase	CEF (SLN)	(27)(14)(12)	(Cr,Fe,Si)(Mo)(Cr,Fe,Mo)
Re24Ti5	CEF (ST2)	(24)(5)	(Re)(Ti)
Re2O7	CEF (ST2)	(2)(7)	(Re)(O)
Re2Si	CEF (ST2)	(2)(1)	(Re)(Si)
Re3B	CEF (SLN)	(0.75)(0.25)	(Mo,Re)(B)
Re7B3	CEF (SLN)	(0.3)(0.7)	(B)(Mo,Re)
ReB2	CEF (SLN)	(1)(2)	(B,Re)(B)
ReO2	CEF (ST2)	(1)(2)	(Re)(O)
ReO3	CEF (ST2)	(1)(3)	(Re)(O)
ReSi	CEF (SLN)	(1)(1)	(Mn,Re)(Si)
ReTi	CEF (ST2)	(1)(1)	(Re)(Ti)
Rutile	CEF (SLN)	(1)(2)	(Mn+4,Ti+3,Ti+4)(O-2,Va)
Shp_MC	CEF (ST2)	(1)(1)	(Mo)(C)
Si2Ti	CEF (SLN)	(2)(1)	(Si)(Mo,Ti)
Si2Zr	CEF (SLN)	(2)(1)	(Si)(Hf,Zr)
Si3Ti5	CEF (SLN)	(0.375)(0.625)	(Si)(Hf,Mn,Mo,Ti,Zr)
Si4Ti5	CEF (SLN)	(4)(5)	(Si)(Hf,Mo,Ti,Zr)
SiC	CEF (ST2)	(1)(1)	(C)(Si)
SiO_AM	CEF (ST2)	(1)(1)	(Si)(O)
SiTi3	CEF (SLN)	(1)(3)	(Si)(Ti,Zr)
Sigma	CEF (SLN)	(10)(4)(16)	(Al,Fe,Mn,Re,Si)(Cr,Fe,Mo,Re) (Al,Cr,Fe,Mn,Mo,Re,Si)
Spinel	CEF (SLN)	(1)(2)(2)(4)	(Al+3,Cr+2,Cr+3,Fe+2,Fe+3) (Al+3,Cr+3,Fe+2,Fe+3,Va)

Name	Model	Lattice Size	Constituent
			(Fe+2,Va)(O-2)
T_AlFeMo	CEF (SLN)	(1)	(Al,Fe,Mo)
Ti10O19	CEF (ST2)	(10)(19)	(Ti)(O)
Ti20O39	CEF (ST2)	(20)(39)	(Ti)(O)
Ti3O2	CEF (ST2)	(3)(2)	(Ti)(O)
Ti3O5	CEF (ST2)	(3)(5)	(Ti)(O)
Ti4O7	CEF (ST2)	(4)(7)	(Ti)(O)
Ti5O9	CEF (ST2)	(5)(9)	(Ti)(O)
Ti6O11	CEF (ST2)	(6)(11)	(Ti)(O)
Ti6Si2B	CEF (ST3)	(6)(2)(1)	(Ti)(Si)(B)
Ti7O13	CEF (ST2)	(7)(13)	(Ti)(O)
Ti8O15	CEF (ST2)	(8)(15)	(Ti)(O)
Ti9O17	CEF (ST2)	(9)(17)	(Ti)(O)
TiOx	CEF (SLN)	(1)(1)(1)	(Ti+2,Ti+3,Va)(Ti,Va)(O-2)
Tridymite	CEF (ST2)	(1)(2)	(Si)(O)
VO2	CEF (SLN)	(1)(2)	(Hf,Mo,Zr)(O)
Y2O3_cub	CEF (SLN)	(2)(3)(1)	(Mn+3,Va)(O-2)(O-2,Va)
Y2O3_hex	CEF (SLN)	(2)(3)(1)	(Zr+4)(O-2)(O-2,Va)
Zr2O	CEF (ST2)	(2)(1)	(Zr)(O)
Zr3O	CEF (ST2)	(3)(1)	(Zr)(O)
Zr6O	CEF (ST2)	(6)(1)	(Zr)(O)
ZrB12	CEF (ST2)	(1)(12)	(Zr)(B)
ZrO2_Cubic	CEF (SLN)	(1)(2)	(Hf,Zr)(O,Va)
ZrO2_Tetra-gonal	CEF (SLN)	(1)(2)	(Hf,Zr)(O,Va)