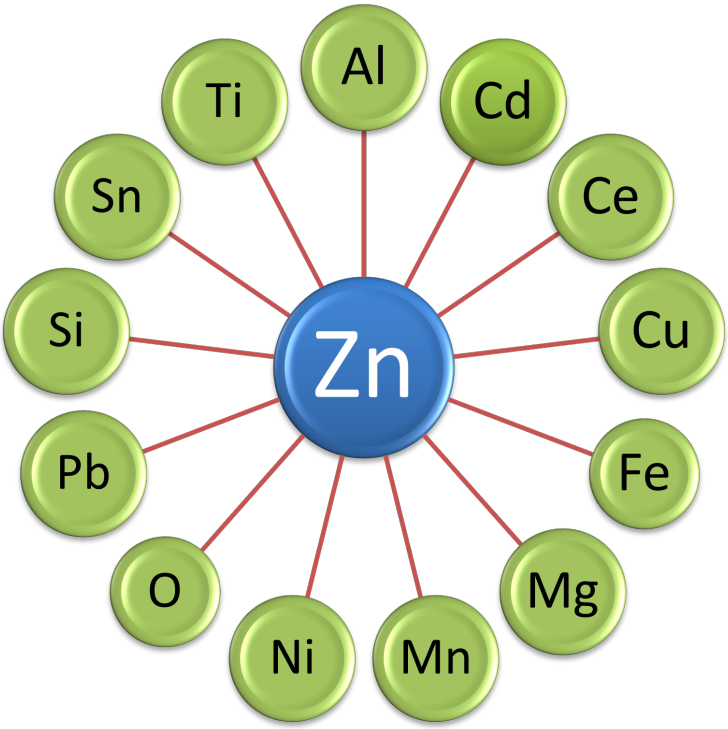
Pandat™ 2024

Database Manual

CompuTherm LLC

PanZinc

Database for multi-component zinc alloys



PANDAT™
SOFTWARE

Contents

1 Thermodynamic Database

1.1 Components (14)

Total of **14** components are included in the database as listed here:

Elements: Al, Cd, Ce, Cu, Fe, Mg, Mn, Ni, O, Pb, Si, Sn, Ti, **Zn**

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.%)
Al	0 ~ 80
Mg	0 ~ 40
Cu, Fe, Mn, Ni, Si	0 ~ 10
Ce, Pb, Sn, Ti	0 ~ 2
Cd, O	0 ~ 0.5
Zn	Balance

1.3 What is new in PanZn2024

Addition of the component O.

1.4 Phases

Total of **325** 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 through TDB viewer of Pandat™.

Table 1.2: Phase name and related information

Name	Lattice Size	Constituent
Al13M4	(0.6275)(0.235) (0.1375)	(Al)(Fe,Mn,Ni,Si,Zn)(Al,Si,Zn,Va)
Al31Mn8Zn11	(0.62)(0.16) (0.22)	(Al)(Mn)(Zn)
Al3Ni8Zn9	(3)(8)(9)	(Al)(Ni)(Zn)
Bcc	(1)(3)	(Al,Cd,Ce,Cu,Fe,Mg,Mn,Ni,Pb,Si,Sn,Ti,Zn)(O,Va)
Bcc_B2	(0.5)(0.5)(3)	(Al,Fe,Mg,Mn,Ni,Si,Ti)(Al,Fe,Mg,Mn,Ni,Si,Ti)(Va)
Fcc	(1)(1)	(Al,Cd,Ce,Cu,Fe,Mg,Mn,Ni,Pb,Si,Sn,Ti,Zn)(O,Va)
Hcp	(1)(0.5)	(Al,Cd,Ce,Cu,Fe,Mg,Mn,Ni,Pb,Si,Sn,Ti,Zn)(O,Va)
Laves_C14	(2)(1)	(Al,Fe,Mg,Mn,Ni,Si,Ti,Zn) (Al,Fe,Mg,Mn,Ni,Si,Ti,Zn)
Laves_C15	(2)(1)	(Al,Cu,Fe,Mg,Mn,Ni,Si,Ti,Zn) (Al,Ce,Cu,Fe,Mg,Mn,Ni,Si,Ti,Zn)
Liquid	(1)	(Al,Cd,Ce,Cu,Fe,Mg,Mg2Sn,Mn,Ni,Pb,Si,Sn,Ti,Zn)

1.5 Assessed Subsystems

A total of **118** subsystems, including 86 binary and 32 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 (86)

Al-Cd(10)	Al-Ce(10)	Al-Cu(10)	Al-Fe(10)	Al-Mg(10)	Al-Mn(10)	Al-Ni(10)
Al-O(10)	Al-Pb(10)	Al-Si(10)	Al-Sn(10)	Al-Ti(10)	Al-Zn(10)	Cd-Ce(10)
Cd-Cu(10)	Cd-Fe(10)	Cd-Mg(10)	Cd-Mn(10)	Cd-Ni(10)	Cd-Pb(10)	Cd-Si(10)
Cd-Sn(10)	Cd-Ti(10)	Cd-Zn(10)	Ce-Cu(10)	Ce-Fe(10)	Ce-Mg(10)	Ce-Mn(10)
Ce-Ni(10)	Ce-O(10)	Ce-Si(10)	Ce-Ti(10)	Ce-Zn(10)	Cu-Fe(10)	Cu-Mg(10)
Cu-Mn(10)	Cu-Ni(10)	Cu-O(10)	Cu-Pb(10)	Cu-Si(10)	Cu-Sn(10)	Cu-Ti(10)
Cu-Zn(10)	Fe-Mg(10)	Fe-Mn(10)	Fe-Ni(10)	Fe-O(10)	Fe-Pb(10)	Fe-Si(10)
Fe-Sn(10)	Fe-Ti(10)	Fe-Zn(10)	Mg-Mn(10)	Mg-Ni(10)	Mg-O(10)	Mg-Si(10)
Mg-Sn(10)	Mg-Ti(10)	Mg-Zn(10)	Mn-Ni(10)	Mn-O(10)	Mn-Pb(10)	Mn-Si(10)
Mn-Sn(10)	Mn-Ti(10)	Mn-Zn(10)	Ni-O(10)	Ni-Pb(10)	Ni-Si(10)	Ni-Sn(10)
Ni-Ti(10)	Ni-Zn(10)	O-Pb(10)	O-Si(10)	O-Sn(10)	O-Ti(10)	O-Zn(5)
Pb-Si(10)	Pb-Sn(10)	Pb-Zn(10)	Si-Sn(10)	Si-Ti(10)	Si-Zn(10)	Sn-Ti(10)
Sn-Zn(10)	Ti-Zn(10)					

Ternary Systems (32)

Al-Ce-Fe(10)	Al-Ce-Mn(10)	Al-Ce-Si(10)	Al-Ce-Zn(10)	Al-Fe-Ni(10)	Al-Fe-Si(10)
Al-Fe-Ti(10)	Al-Fe-Zn(10)	Al-Mg-Mn(10)	Al-Mg-Si(10)	Al-Mg-Ti(10)	Al-Mg-Zn(10)
Al-Mn-Ni(10)	Al-Mn-Si(10)	Al-Mn-Ti(10)	Al-Ni-Si(10)	Al-Ni-Ti(10)	Al-Si-Ti(10)
Al-Si-Zn(10)	Fe-Mg-Mn(10)	Fe-Mg-Si(10)	Fe-Mn-Si(10)	Fe-Mn-Ti(10)	Fe-Mn-Zn(10)
Fe-Ni-Si(10)	Fe-Ni-Ti(10)	Mg-Mn-Ni(10)	Mg-Mn-Si(10)	Mn-Ni-Si(10)	Mn-Si-Zn(10)
Ni-Si-Ti(10)	Ni-Si-Zn(10)				

1.6 Database Validation and Application

The PanZn database is the commercial database for alloy design and processing optimization of Zn alloys. It has been validated by a large amount of experimental data.

Berent et al [2016Ber]did the thermal analysis and microstructure observation of a serial of Zn-Al-Si alloys. The microstructure shows primary Si particles, Zn+Al eutectic structure and Zn+Al eutectoid structure. Figure 1.1 shows the calculated phase diagram of Zn-5.3Al-xSi (wt.%) section. The calculated result is in good agreement with their thermal analysis results and microstructure observations.

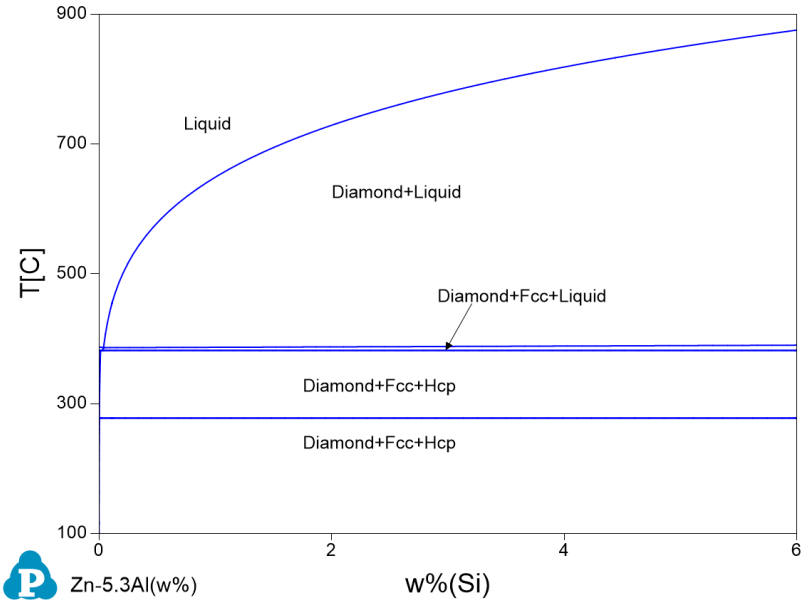


Figure 1.1: Calculated phase diagram of Zn-5.3Al-xSi (wt.%) section.

Gogola et al. [2021Gog] measured the liquidus and solidus temperatures of a serial Zn-Al-Mg-Sn alloys. The calculated results using this database is in good agreement with the experimental data as shown in Figure 1.2.

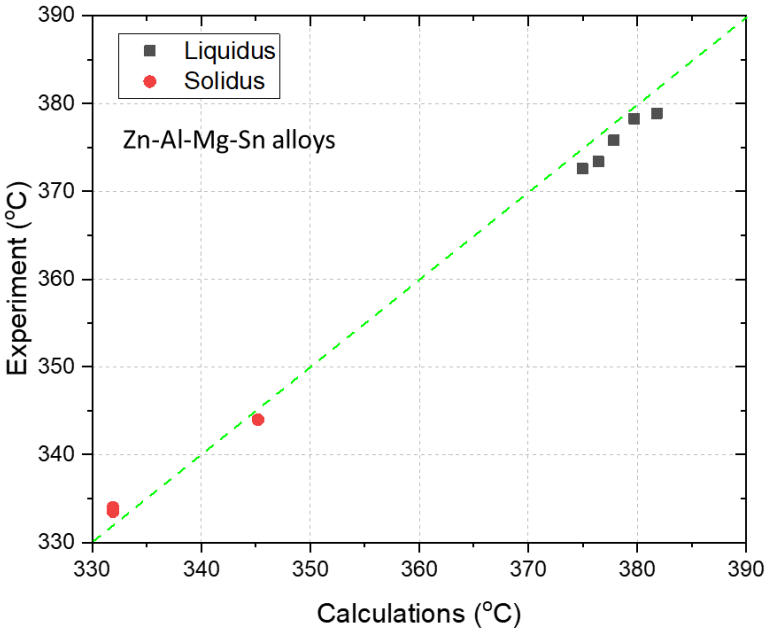


Figure 1.2: The comparison of the liquidus and solidus temperature of Zn-Al-Mg-Sn alloys from experiments and calculations

2 Mobility Database

PanZn2024_MB is an atomic mobility database for zinc alloys, which is compatible with the `PanZn2024_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	Cd	Ce	Cu	Fe	Mg	Mn	Ni	Pb	Si	Sn	Ti	Zn
Bcc													
Fcc													
Hcp													

2.3 Assessed Systems

In addition to the assessed self-diffusivities shown above, the impurity diffusion data for all included elements in the current `PanZn2024_MB` database are also assessed. In the following, the assessed chemical-diffusivity within the binary and ternary systems for the **Bcc** , **Fcc** and **Hcp** phases are listed, respectively.

Fcc Phase

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

Cu-Zn Fe-Mn Fe-Ni Fe-Zn Ni-Zn

Al-Cu-Mg Al-Mg-Zn Cu-Fe-Mn Cu-Fe-Ni Cu-Ni-Mn Cu-Ni-Zn

Bcc phase

Al-Fe Al-Ti Cu-Ti Ni-Ti

Hcp phase

Al-Mg Al-Zn Cd-Zn Mg-Sn Mg-Zn

Al-Mg-Sn Al-Mg-Zn

2.4 Database Validation

The simulated concentration profiles of a series of zinc alloys are shown below to validate the current `PanZn2024_MB` database.

Figure 2.1 shows the calculated self-diffusion of Zn and inter-diffusion coefficients of Zn within the Hcp Zn-X (X=Cu, Cd, Sn) binary systems using the current `PanZn_MB` database. The calculated results are in good agreement with the experimental data.

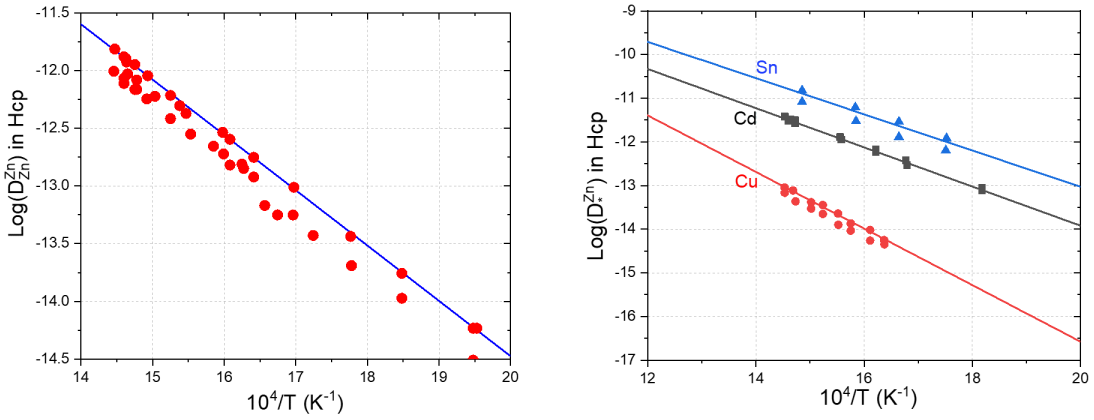


Figure 2.1: left: self-diffusivity of pure Zn; right: inter-diffusion coefficients of Zn-X (X=Cu, Cd, Sn) systems in Hcp phase.

Figure 2.2 shows the simulated concentration profiles of Cu-Zn binary system aged at 380 °C for 25h.

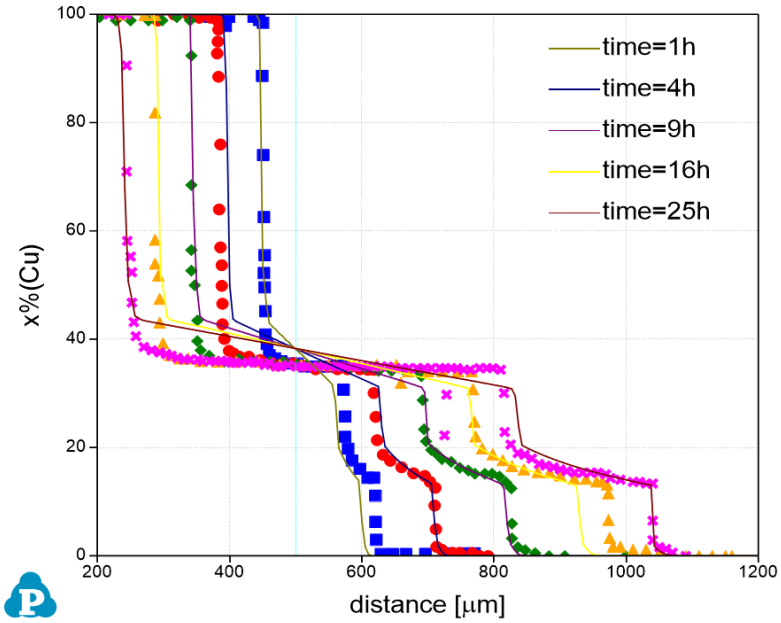


Figure 2.2: Concentration profiles of Cu-Zn (at.%) aged at 380°C for 25h

3 Thermophysical Property Database

The thermophysical property database **PanZn2024_TP** is compatible with the `PanZn2024_TH` thermodynamic database and suitable for the simulation of thermophysical properties of Zn-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 **325** phases assessed in the `PanZn2024_TH` database. It is used to calculate the density, thermal expansion and solidification shrinkage of Zn alloys.

Figure 3.1 shows the molar volume of Zn together with experimental data. Figure 3.2 shows the molar volume of Al-Zn Fcc binary alloys at 298K. The calculated results agree well with the experimental data.

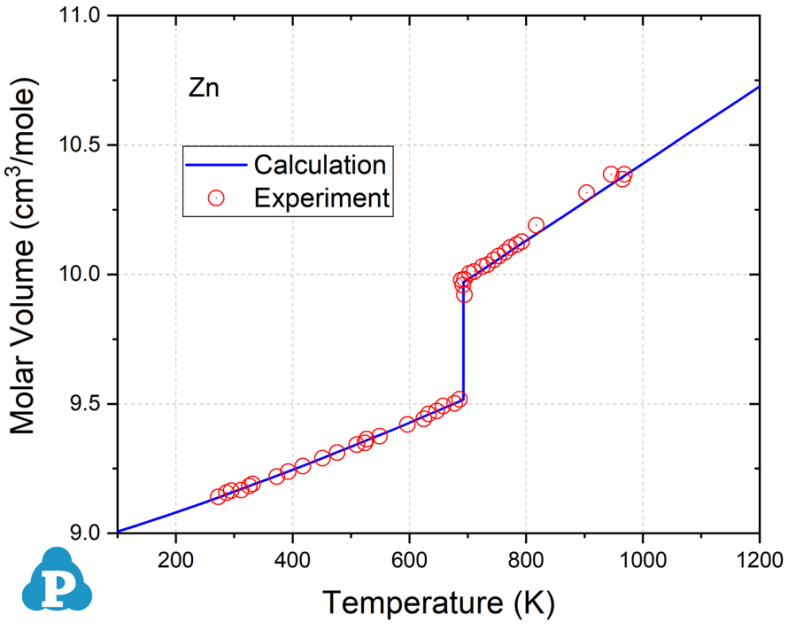


Figure 3.1: Molar volume of Zn

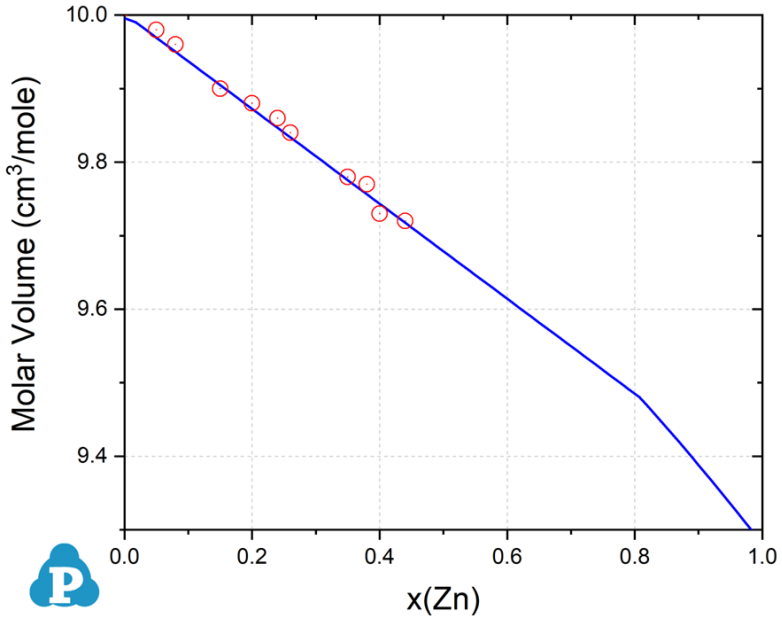


Figure 3.2: Molar volume of Al-Zn Fcc binary alloys at 298K

3.2 Surface Tension

The surface tension of the liquid phase is included in the property database. Figure 3.3 shows the surface tension of a series of Zn-Li alloys in comparison with experimental data.

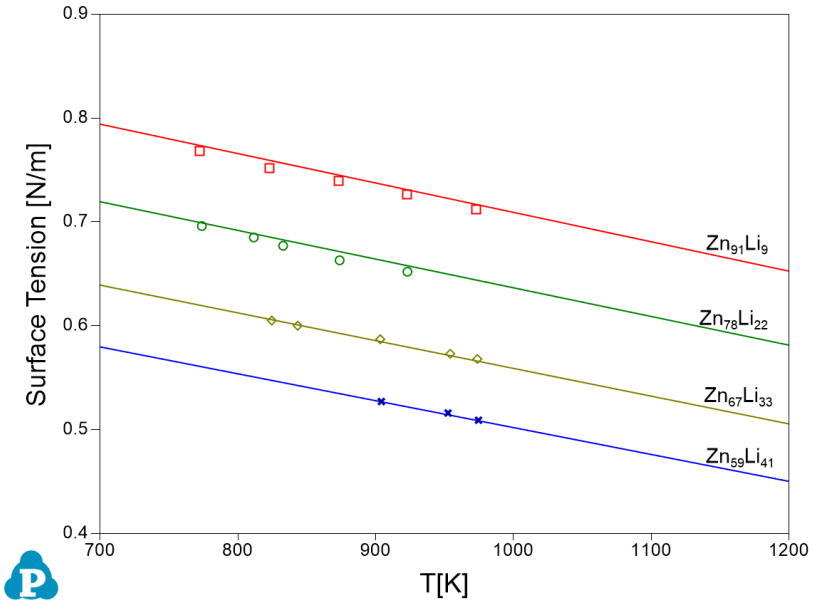


Figure 3.3: Surface tension of Zn-Li alloys

3.3 Viscosity

The viscosity of the liquid phase is included in the property database. Figure 3.4 shows the viscosity of Zn-9at.% Li alloy in comparison with experimental data.

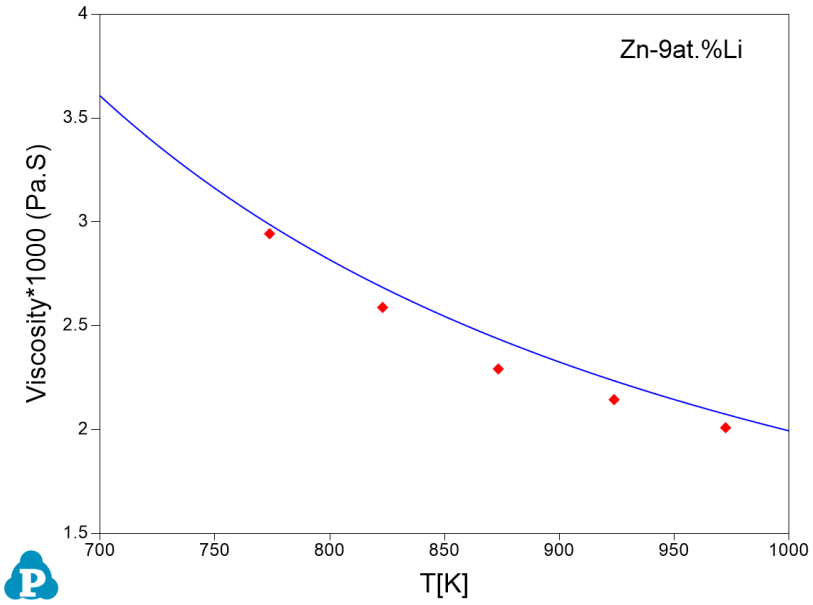


Figure 3.4: Viscosity of the Zn-9Li alloy

4 References

[2016Ber] K. Berent, J. Pstruś, T. Gancarz, Thermal and Microstructure Characterization of Zn-Al-Si Alloys and Chemical Reaction with Cu Substrate During Spreading, J. Mater. Eng. Perform., 25 (2016) 3375-3383

[2021Gog] P. Gogola, Z. Gabalcová, M. Kusý, H. Suchánek, The Effect of Sn Addition on Zn-Al-Mg Alloy; Part I: Microstructure and Phase Composition, Materials (Basel), 14 (2021) 5404.

PanZn2024: List of Phases

Phases (**325**)

Name	Model	Lattice Size	Constituent
Name	Model	Lattice Size	Constituent
A15	CEF (SLN)	(0.75)(0.25) (0.05)	(Fe,Si,Ti)(Al,Ni,Si,Ti)(Va)
A_RE2O3	CEF (SLN)	(2)(2)(1)	(Ce+3,Ce+2)(O-2)(O-2,Va)
A_TiO	CEF (ST2)	(1)(1)	(Ti)(O)
Al10CeFe2	CEF (ST3)	(10)(1)(2)	(Al)(Ce)(Fe)
Al10Fe3Ni	CEF (ST3)	(10)(3)(1)	(Al)(Fe)(Ni)
Al10FeNi3	CEF (ST3)	(10)(1)(3)	(Al)(Fe)(Ni)
Al11Mn4_H	CEF (SLN)	(29)(10)	(Al,Mn)(Mn)
Al11Mn4_L	CEF (SLN)	(11)(4)	(Al,Zn)(Mn)
Al12Mn	CEF (ST2)	(12)(1)	(Al)(Mn)
Al13CeMg6	CEF (ST3)	(13)(1)(6)	(Al)(Ce)(Mg)

Name	Model	Lattice Size	Constituent
Al13M4	CEF (SLN)	(0.6275) (0.235) (0.1375)	(Al)(Fe,Mn,Ni,Si,Zn)(Al,Si,Zn,Va)
Al14Mn4Si5	CEF (SLN)	(14)(4)(5)	(Al)(Mn)(Al,Si)
Al15_FeMn3Si2	CEF (SLN)	(16)(4)(1) (2)	(Al)(Fe,Mn)(Si)(Al,Si)
Al16Ce10Si4	CEF (ST3)	(0.533333) (0.333333) (0.133333)	(Al)(Ce)(Si)
Al18Mg3X2	CEF (SLN)	(18)(3)(2)	(Al)(Mg)(Mn,Ti)
Al1Fe1O3	CEF (ST3)	(1)(1)(3)	(Al+3)(Fe+3)(O-2)
Al2CeSi2	CEF (SLN)	(0.666667) (0.333333)	(Al,Si)(Ce)
Al2CeZn2	CEF (ST3)	(2)(1)(2)	(Al)(Ce)(Zn)
Al2Fe	CEF (SLN)	(2)(1)	(Al,Si,Zn)(Fe,Mn)
Al2Mn2Si3	CEF (ST3)	(2)(2)(3)	(Al)(Mn)(Si)
Al2MnSi3	CEF (ST3)	(2)(1)(3)	(Al)(Mn)(Si)
Al2Ti	CEF (SLN)	(2)(1)	(Al,Ti)(Al,Ti)
Al31Mn8Zn11	CEF	(0.62)(0.16)	(Al)(Mn)(Zn)

Name	Model	Lattice Size	Constituent
	(ST3)	(0.22)	
Al3Mn4Si2	CEF (ST3)	(3)(4)(2)	(Al)(Mn)(Si)
Al3MnSi2	CEF (ST3)	(3)(1)(2)	(Al)(Mn)(Si)
Al3Ni	CEF (ST2)	(0.75)(0.25)	(Al)(Ni)
Al3Ni5	CEF (ST2)	(0.375) (0.625)	(Al)(Ni)
Al3Ni8Zn9	CEF (ST3)	(3)(8)(9)	(Al)(Ni)(Zn)
Al3NiM2	CEF (SLN)	(3)(2)(1)	(Al,Si)(Al,Ni)(Ni,Va)
Al4Ce	CEF (ST2)	(0.8)(0.2)	(Al)(Ce)
Al4CeMg4	CEF (ST3)	(4)(1)(4)	(Al)(Ce)(Mg)
Al4Mn4Si2	CEF (SLN)	(0.8)(0.2)	(Al,Mn)(Si)
Al4Mn_R	CEF (ST2)	(461)(107)	(Al)(Mn)
Al4Mn_U	CEF (SLN)	(0.2)(0.8)	(Fe,Mn)(Al,Zn,Va)
Al5Fe2	CEF (SLN)	(5)(2)(3)	(Al,Si)(Fe,Mn,Ni)(Zn,Va)
Al5Fe4	CEF	(1)	(Al,Fe,Mn)

Name	Model	Lattice Size	Constituent
	(SLN)		
Al5Mn2Si5	CEF (ST3)	(0.7)(0.2) (0.1)	(Al)(Mn)(Si)
Al5Mn6Si7	CEF (ST3)	(5)(6)(7)	(Al)(Mn)(Si)
Al5Ti2	CEF (SLN)	(5)(2)	(Al,Ti)(Al,Ti)
Al5Ti3	CEF (ST2)	(5)(3)	(Al)(Ti)
Al6Mn	CEF (ST2)	(6)(1)	(Al)(Mn)
Al6Ni3Si	CEF (ST3)	(6)(3)(1)	(Al)(Ni)(Si)
Al71Mn16Zn13	CEF (ST3)	(0.71)(0.16) (0.13)	(Al)(Mn)(Zn)
Al8CeFe2	CEF (ST3)	(8)(1)(2)	(Al)(Ce)(Fe)
Al8FeMg3Si6	CEF (ST4)	(8)(3)(1)(6)	(Al)(Mg)(Fe)(Si)
Al8FeMnSi2	CEF (ST4)	(16)(2)(2) (3)	(Al)(Fe)(Mn)(Si)
Al8Mn5	CEF (SLN)	(0.4615) (0.1923) (0.3462)	(Al)(Fe,Mn)(Al,Fe,Mn,Si,Ti,Zn)
Al8RM4	CEF (SLN)	(8)(1)(4)	(Al)(Ce)(Fe,Mn)

Name	Model	Lattice Size	Constituent
Al9FeNi	CEF (ST3)	(9)(1)(1)	(Al)(Fe)(Ni)
AlCe2	CEF (ST2)	(1)(2)	(Al)(Ce)
AlCeSi2	CEF (ST3)	(0.25)(0.25) (0.5)	(Al)(Ce)(Si)
AlCu_Delta	CEF (ST2)	(0.4)(0.6)	(Al)(Cu)
AlCu_Eps	CEF (SLN)	(0.5)(0.5)	(Al,Cu)(Cu)
AlCu_Eta	CEF (SLN)	(0.5)(0.5)	(Al,Cu)(Cu)
AlCu_Gamma	CEF (SLN)	(1)(1)	(Al,Cu,Mn,Si)(Va)
AlCu_Theta	CEF (SLN)	(0.667) (0.333)	(Al)(Al,Cu,Ti)
AlCu_Zeta	CEF (ST2)	(0.45)(0.55)	(Al)(Cu)
AlFeTi_T1	CEF (ST3)	(0.25)(0.5) (0.25)	(Al)(Fe)(Ti)
AlFeTi_T2	CEF (ST3)	(0.53448) (0.25172) (0.2138)	(Al)(Fe)(Ti)
AlFeTi_T3	CEF (ST3)	(0.65) (0.075) (0.275)	(Al)(Fe)(Ti)
AlFeTi_T4	CEF	(0.35)(0.23)	(Al)(Fe)(Ti)

Name	Model	Lattice Size	Constituent
	(ST3)	(0.42)	
AlMg_Beta	CEF (SLN)	(89)(140)	(Mg)(Al,Zn)
AlMg_Eps	CEF (SLN)	(23)(30)	(Mg)(Al,Zn)
AlMg_Gamma	CEF (SLN)	(10)(24)(24)	(Mg)(Al,Mg,Zn)(Al,Mg,Zn)
AlMnSi	CEF (ST3)	(1)(1)(1)	(Al)(Mn)(Si)
AlNi16Si9	CEF (ST3)	(1)(16)(9)	(Al)(Ni)(Si)
AlNi2Si	CEF (SLN)	(1)(1)	(Ni)(Al,Si,Va)
AlNi2Zn	CEF (ST3)	(1)(2)(1)	(Al)(Ni)(Zn)
AlNiTi_T1	CEF (ST3)	(0.65)(0.1) (0.25)	(Al)(Ni)(Ti)
AlNiTi_T2	CEF (SLN)	(0.5517) (0.2069) (0.2414)	(Al,Ti)(Ti)(Ni)
Alpha_AlFeSi	CEF (SLN)	(0.66)(0.19) (0.05)(0.1)	(Al)(Fe)(Si)(Al,Si)
Alpha_TiMn	CEF (ST2)	(1)(1)	(Mn)(Ti)
B2	CEF (SLN)	(1)(1)	(Al,Fe,Mg,Mn,Ni,Si,Ti,Zn) (Ce,Fe,Mn,Ni,Si,Ti,Va)

Name	Model	Lattice Size	Constituent
BCT_A5	CEF (SLN)	(1)	(Al,Cd,Cu,Ni,Pb,Sn,Zn)
Bcc	CEF (SLN)	(1)(3)	(Al,Cd,Ce,Cu,Fe,Mg,Mn,Ni,Pb,Si,Sn, Ti,Zn)(O,Va)
Bcc_B2	CEF (SLN)	(0.5)(0.5)(3)	(Al,Fe,Mg,Mn,Ni,Si,Ti) (Al,Fe,Mg,Mn,Ni,Si,Ti)(Va)
Beta_AlFeSi	CEF (SLN)	(0.598) (0.152)(0.1) (0.15)	(Al)(Fe,Mn)(Si)(Al,Si)
Beta_TiMn	CEF (ST2)	(0.515) (0.485)	(Mn)(Ti)
CBCC_A12	CEF (SLN)	(1)(1)	(Al,Ce,Cu,Fe,Mn,Ni,Si,Sn,Ti,Zn)(Va)
CUB_A13	CEF (SLN)	(1)(1)	(Al,Ce,Cu,Fe,Mg,Mn,Ni,Si,Sn,Ti,Zn)(Va)
C_Ce2O3	CEF (SLN)	(2)(3)(1)	(Ce+3,Ce+4)(O-2)(O-2,Va)
Cd10Cu3	CEF (ST2)	(0.7692) (0.2308)	(Cd)(Cu)
Cd11Ce	CEF (ST2)	(11)(1)	(Cd)(Ce)
Cd17Ce2	CEF (ST2)	(17)(2)	(Cd)(Ce)
Cd2Ce	CEF (ST2)	(2)(1)	(Cd)(Ce)
Cd3Ce	CEF (ST2)	(3)(1)	(Cd)(Ce)

Name	Model	Lattice Size	Constituent
Cd3Cu4	CEF (ST2)	(0.4268) (0.5714)	(Cd)(Cu)
Cd58Ce13	CEF (ST2)	(58)(13)	(Cd)(Ce)
Cd5Ni	CEF (SLN)	(0.83)(0.17)	(Cd)(Cd,Ni)
Cd6Ce	CEF (ST2)	(6)(1)	(Cd)(Ce)
Cd8Cu5	CEF (SLN)	(0.6154) (0.3846)	(Cd,Cu)(Cd,Cu)
CdCe	CEF (ST2)	(0.5)(0.5)	(Cd)(Ce)
CdCu2	CEF (ST2)	(0.33333) (0.66667)	(Cd)(Cu)
CdMg_order	CEF (SLN)	(0.25)(0.25) (0.25)(0.25) (0.5)	(Cd,Mg)(Cd,Mg)(Cd,Mg)(Cd,Mg)(Va)
CdNi	CEF (SLN)	(0.5)(0.5)	(Cd)(Cd,Ni)
CdSn_Beta	CEF (SLN)	(1)	(Cd,Sn)
CdTi	CEF (ST2)	(0.5)(0.5)	(Ti)(Cd)
CdTi2	CEF (ST2)	(0.6667) (0.3333)	(Ti)(Cd)
Ce11O20	CEF (ST2)	(11)(20)	(Ce)(O)

Name	Model	Lattice Size	Constituent
Ce13Zn58	CEF (ST2)	(0.183) (0.817)	(Ce)(Zn)
Ce19O34	CEF (ST2)	(19)(34)	(Ce)(O)
Ce2Fe17	CEF (SLN)	(2)(17)	(Ce)(Al,Fe)
Ce2Mg17	CEF (ST2)	(2)(17)	(Ce)(Mg)
Ce2Mg53Zn45	CEF (ST3)	(2)(53)(45)	(Ce)(Mg)(Zn)
Ce2Zn17	CEF (ST2)	(0.105) (0.895)	(Ce)(Zn)
Ce3Si2	CEF (ST2)	(0.6)(0.4)	(Ce)(Si)
Ce3Si5	CEF (ST2)	(0.375) (0.625)	(Ce)(Si)
Ce3Zn11	CEF (ST2)	(0.214) (0.786)	(Ce)(Zn)
Ce3Zn22	CEF (ST2)	(0.12)(0.88)	(Ce)(Zn)
Ce40O72	CEF (ST2)	(40)(72)	(Ce)(O)
Ce5Mg41	CEF (ST2)	(5)(41)	(Ce)(Mg)
Ce5Si3	CEF (ST2)	(0.625) (0.375)	(Ce)(Si)

Name	Model	Lattice Size	Constituent
Ce5Si4	CEF (ST2)	(0.555556) (0.444444)	(Ce)(Si)
Ce62O112	CEF (ST2)	(62)(112)	(Ce)(O)
Ce7Ni3	CEF (ST2)	(0.7)(0.3)	(Ce)(Ni)
Ce7O12	CEF (ST2)	(7)(12)	(Ce)(O)
Ce9O16	CEF (ST2)	(9)(16)	(Ce)(O)
CeFe2	CEF (ST2)	(1)(2)	(Ce)(Fe)
CeMg	CEF (SLN)	(0.5)(0.5)	(Ce)(Al,Mg)
CeMg12	CEF (SLN)	(1)(12)	(Ce)(Al,Mg,Zn)
CeMg2	CEF (ST2)	(0.333333) (0.666667)	(Ce)(Mg)
CeMg3	CEF (SLN)	(1)(3)	(Ce)(Mg,Zn)
CeMg3Zn5	CEF (ST3)	(1)(3)(5)	(Ce)(Mg)(Zn)
CeMg7Zn12	CEF (ST3)	(1)(7)(12)	(Ce)(Mg)(Zn)
CeNi	CEF (ST2)	(0.5)(0.5)	(Ce)(Ni)

Name	Model	Lattice Size	Constituent
CeNi2	CEF (ST2)	(0.3333) (0.6667)	(Ce)(Ni)
CeNi3	CEF (ST2)	(0.25)(0.75)	(Ce)(Ni)
CeNi5	CEF (ST2)	(0.1667) (0.8333)	(Ce)(Ni)
CeSi	CEF (ST2)	(0.5)(0.5)	(Ce)(Si)
CeSi2	CEF (ST2)	(0.333333) (0.666667)	(Ce)(Si)
CeZn11	CEF (ST2)	(0.083) (0.917)	(Ce)(Zn)
CeZn2	CEF (ST2)	(0.333) (0.667)	(Ce)(Zn)
CeZn3	CEF (ST2)	(0.25)(0.75)	(Ce)(Zn)
CeZn5	CEF (ST2)	(0.167) (0.833)	(Ce)(Zn)
Corundum	CEF (SLN)	(2)(1)(3)	(Al+3,Fe+2,Fe+3,Ti+3,Va) (Fe+3,Ni+2,Va)(O-2)
Cristobalite	CEF (ST2)	(1)(2)	(Si)(O)
Cu10Sn3	CEF (SLN)	(1)	(Cu,Sn)
Cu2Ce	CEF (ST2)	(0.666667) (0.333333)	(Cu)(Ce)

Name	Model	Lattice Size	Constituent
Cu2O	CEF (ST2)	(2)(1)	(Cu)(O)
Cu2Ti	CEF (SLN)	(0.666667) (0.333333)	(Cu,Fe,Ni)(Ti)
Cu3Sn	CEF (SLN)	(3)(1)	(Cu,Sn)(Cu,Sn)
Cu3Ti2	CEF (SLN)	(0.6)(0.4)	(Cu,Fe,Ni)(Ti)
Cu41Sn11	CEF (SLN)	(41)(11)	(Cu,Sn)(Cu,Sn)
Cu4Ce	CEF (ST2)	(0.8)(0.2)	(Cu)(Ce)
Cu4Ti	CEF (SLN)	(0.8)(0.2)	(Cu,Ni,Ti)(Cu,Ni,Ti)
Cu4Ti3	CEF (SLN)	(0.57143) (0.42857)	(Cu,Fe,Ni)(Ti)
Cu5Ce	CEF (ST2)	(0.833333) (0.166667)	(Cu)(Ce)
Cu6Ce	CEF (ST2)	(0.857143) (0.142857)	(Cu)(Ce)
Cu6Sn5_L	CEF (SLN)	(1)(1)(1)	(Cu)(Cu,Sn,Va)(Sn)
CuCe	CEF (ST2)	(0.5)(0.5)	(Ce)(Cu)
CuMg2	CEF (SLN)	(0.33333) (0.66667)	(Cu,Ni)(Mg)

Name	Model	Lattice Size	Constituent
CuO	CEF (ST2)	(1)(1)	(Cu)(O)
CuSn_Gamma	CEF (SLN)	(1)	(Cu,Mg,Mn,Sn)
CuTi	CEF (SLN)	(0.5)(0.5)	(Cu,Ni,Ti)(Cu,Ni,Ti)
CuTi2	CEF (SLN)	(1)(2)	(Cu,Fe,Ni)(Al,Ti)
CuZn_Beta	CEF (SLN)	(1)	(Cu,Zn)
D0_19	CEF (SLN)	(0.75)(0.25) (0.5)	(Al,Mn,Ni,Ti)(Al,Mn,Ni,Si,Ti)(Va)
D0_22	CEF (SLN)	(3)(1)	(Al,Si,Ti)(Al,Ti)
D0_22_TiAl3_L	CEF (SLN)	(3)(1)	(Al,Ti)(Al,Ti)
Delta_AlFeSi	CEF (SLN)	(5)(1)	(Al,Si)(Fe)
Delta_Cu33Si7	CEF (SLN)	(0.825) (0.175)	(Cu,Mg)(Si)
Diamond	CEF (SLN)	(1)	(Al,Ni,Si)
Eps	CEF (SLN)	(1)	(Al,Cu,Zn)
Epsilon_ Cu15Si4	CEF (SLN)	(0.789474) (0.210526)	(Cu,Mg,Zn)(Al,Si)

Name	Model	Lattice Size	Constituent
Eta_Cu19Si6	CEF (SLN)	(0.76)(0.24)	(Cu,Mg)(Si)
F_Ce2O4	CEF (SLN)	(2)(4)	(Ce+3,Ce+4)(O-2,Va)
Fcc	CEF (SLN)	(1)(1)	(Al,Cd,Ce,Cu,Fe,Mg,Mn,Ni,Pb,Si, Sn,Ti,Zn)(O,Va)
Fe2Si	CEF (ST2)	(0.666667) (0.333333)	(Fe)(Si)
Fe2TiZn22	CEF (ST3)	(2)(1)(22)	(Fe)(Ti)(Zn)
Fe3Sn2	CEF (ST2)	(3)(2)	(Fe)(Sn)
Fe5Ni3Si2	CEF (SLN)	(0.8)(0.2)	(Fe,Ni)(Si)
Fe5Sn3	CEF (ST2)	(5)(3)	(Fe)(Sn)
FeMn2Zn7	CEF (ST3)	(0.1)(0.2) (0.7)	(Fe)(Mn)(Zn)
FeSi2_H	CEF (SLN)	(0.3)(0.7)	(Fe)(Al,Si)
FeSi2_L	CEF (SLN)	(1)(2)	(Fe,Ni)(Al,Si)
FeSn	CEF (ST2)	(1)(1)	(Fe)(Sn)
FeSn2	CEF (ST2)	(1)(2)	(Fe)(Sn)

Name	Model	Lattice Size	Constituent
FeZn_Delta	CEF (SLN)	(0.058) (0.18) (0.525) (0.237)	(Fe)(Al,Fe,Mn,Si,Zn)(Zn)(Zn)
FeZn_Gamma	CEF (SLN)	(0.154) (0.154) (0.231) (0.461)	(Fe,Mn,Zn)(Fe,Mn,Zn) (Al,Fe,Mn,Si,Zn)(Zn)
FeZn_Gamma1	CEF (SLN)	(0.137) (0.118) (0.745)	(Fe)(Al,Fe,Mn,Si,Zn)(Mn,Zn)
FeZn_Zeta	CEF (SLN)	(0.072) (0.856) (0.072)	(Fe,Mn,Va)(Al,Zn)(Al,Si,Zn,Va)
GAS	GAS	(1)	(Al,AlO,AlO2,Al2,Al2O,Al2O2,Al2O3,Fe, FeO,FeO2,Fe2,Mg,Mg2,MgO,Mn,O,O2, O3,Pb,Pb2,PbO,Pb2O2,Pb3O3,Pb4O4, Pb5O5,Pb6O6,Sn,Sn2,SnO,SnO2,Si, Si2,Si3,SiO,SiO2,Ti,TiO,TiO2,Zn)
Gamma2	CEF (SLN)	(0.255) (0.745)	(Al,Fe,Mn,Zn)(Zn)
Gamma_AlFeSi	CEF (ST3)	(0.635) (0.205) (0.16)	(Al)(Fe)(Si)
Gamma_ Cu56Si11	CEF (SLN)	(0.835821) (0.164179)	(Cu,Mg,Mn,Zn)(Si)
Gamma_H	CEF	(4)(1)(8)	(Al,Si,Zn)(Al,Cu,Zn)(Cu,Fe,Mn)

Name	Model	Lattice Size	Constituent
	(SLN)		
Gammabrass	CEF (SLN)	(1)	(Al,Cu,Mn,Si,Zn)
H_L21	CEF (SLN)	(0.5)(0.5)(1)	(Al,Fe,Mn,Ni,Ti)(Al,Fe,Mn,Ni,Ti) (Fe,Mn,Ni,Va)
H_RE2O3	CEF (SLN)	(2)(2)(1)	(Ce+3,Ce+2)(O-2)(O-2,Va)
Halite	CEF (SLN)	(1)(1)	(Al+3,Fe+2,Fe+3,Mg+2,Mn+2,Mn+3,Ni+2,Va) (O-2,Va)
Hcp	CEF (SLN)	(1)(0.5)	(Al,Cd,Ce,Cu,Fe,Mg,Mn,Ni,Pb,Si,Sn,Ti,Zn) (O,Va)
L10_TiAl	CEF (SLN)	(1)(1)(2)	(Al,Mn,Ti)(Al,Mn,Ti)(Va)
L12_FCC	CEF (SLN)	(0.75)(0.25)	(Al,Fe,Mn,Ni,Si,Ti)(Al,Fe,Mn,Ni,Si,Ti)
L12_ Ti25Mn9Al66	CEF (ST3)	(0.67)(0.08) (0.25)	(Al)(Mn)(Ti)
Laves_C14	CEF (SLN)	(2)(1)	(Al,Fe,Mg,Mn,Ni,Si,Ti,Zn) (Al,Fe,Mg,Mn,Ni,Si,Ti,Zn)
Laves_C15	CEF (SLN)	(2)(1)	(Al,Cu,Fe,Mg,Mn,Ni,Si,Ti,Zn) (Al,Ce,Cu,Fe,Mg,Mn,Ni,Si,Ti,Zn)
Laves_C36	CEF (SLN)	(2)(1)	(Al,Fe,Mg,Mn,Ni,Si,Ti,Zn) (Al,Fe,Mg,Mn,Ni,Si,Ti,Zn)
Liquid	CEF (SLN)	(1)	(Al,Cd,Ce,Cu,Fe,Mg,Mn,Ni,O,Pb,Si,Sn,Ti,Zn, Al2O3,CeO3/2,CeO2,CuO,Cu2O,Cu2O3,Fe-O, FeO3/2,MgO,Mg2Sn,MnO,Mn2/3O,NiO,PbO,

Name	Model	Lattice Size	Constituent
			SiO2,SnO,SnO2,TiO,TiO3/2,TiO2)
M5X3_hP16	CEF (SLN)	(2)(3)(3)	(Al,Fe,Mn,Ni,Si,Ti)(Al,Ni,Si,Ti)(Fe,Mn,Ni,Ti)
M6Sn5	CEF (SLN)	(1)(1)(1)	(Cu,Ni)(Cu,Sn,Ni,Va)(Sn)
MSi	CEF (SLN)	(0.5)(0.5)	(Fe,Mg,Mn,Ni,Si)(Al,Si)
MSi2	CEF (SLN)	(1)(2)	(Fe,Mn,Ni)(Al,Si)
MX2_cF96	CEF (SLN)	(1)(2)	(Fe,Ni,Si,Ti)(Al,Fe,Ni,Ti)
Mg2M	CEF (SLN)	(0.5)(0.25)(0.25)	(Mg)(Al,Si)(Va)
Mg2Ni	CEF (SLN)	(2)(1)	(Mg)(Ni,Zn)
Mg2SiNi3	CEF (ST3)	(2)(1)(3)	(Mg)(Si)(Ni)
Mg2Sn	CEF (SLN)	(2)(1)	(Mg)(Sn,Zn)
Mg2Zn11	CEF (SLN)	(5)(6)(2)	(Al,Sn,Zn)(Zn)(Mg)
Mg2Zn3	CEF (SLN)	(2)(3)	(Mg)(Al,Zn)
Mg3MnNi2	CEF (ST3)	(3)(1)(2)	(Mg)(Mn)(Ni)
Mg3Ni11Si6	CEF	(3)(11)(6)	(Mg)(Ni)(Si)

Name	Model	Lattice Size	Constituent
	(ST3)		
Mg5Ni17Si7	CEF (SLN)	(5)(17)(7)	(Mg)(Ni,Si)(Ni,Si)
Mg7Zn3	CEF (ST2)	(51)(20)	(Mg)(Zn)
MgNi8Si6	CEF (ST3)	(1)(8)(5.5)	(Mg)(Ni)(Si)
MgZn	CEF (SLN)	(12)(13)	(Mg)(Al,Zn)
Mn11Si19	CEF (SLN)	(11)(19)	(Mn,Ni)(Al,Si)
Mn13NiSi6	CEF (ST3)	(13)(1)(6)	(Mn)(Ni)(Si)
Mn19Sn6	CEF (ST2)	(19)(6)	(Mn)(Sn)
Mn2Ni3Si	CEF (ST3)	(1)(1.56)(0.44)	(Mn)(Ni)(Si)
Mn2NiSi	CEF (SLN)	(2)(1)(1)	(Mn,Ni)(Mn,Ni)(Si)
Mn2O3_CUB	CEF (SLN)	(2)(3)(1)	(Mn+3,Va)(O-2)(O-2,Va)
Mn2Sn	CEF (ST2)	(2)(1)	(Mn)(Sn)
Mn3Ni10Si7	CEF (ST3)	(3)(10)(7)	(Mn)(Ni)(Si)
Mn3Ni2Si	CEF	(3)(2)(1)	(Mn)(Ni)(Si)

Name	Model	Lattice Size	Constituent
	(ST3)		
Mn3Ni9Si8	CEF (ST3)	(3)(9)(8)	(Mn)(Ni)(Si)
Mn3O4_A	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3O4_B	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3Si	CEF (SLN)	(3)(1)	(Fe,Mn,Ni)(Al,Si)
Mn3Ti	CEF (ST2)	(3)(1)	(Mn)(Ti)
Mn4Ti	CEF (ST2)	(0.815) (0.185)	(Mn)(Ti)
Mn52Ni29Si19	CEF (ST3)	(52)(29)(19)	(Mn)(Ni)(Si)
Mn61Ni12Si27	CEF (ST3)	(61)(12)(27)	(Mn)(Ni)(Si)
Mn6Ni16Si7	CEF (ST3)	(6)(16)(7)	(Mn)(Ni)(Si)
Mn6Si	CEF (SLN)	(0.85)(0.15)	(Al,Mn)(Si)
Mn9Si2	CEF (ST2)	(0.825) (0.175)	(Mn)(Si)
MnNi2	CEF (SLN)	(1)(2)	(Mn,Ni)(Ni)
MnNiSi	CEF	(1)(1)(1)	(Mn)(Ni)(Si)

Name	Model	Lattice Size	Constituent
	(ST3)		
MnNiSi_P	CEF (SLN)	(1)(1)(1)	(Mn)(Ni)(Ni,Si)
MnNi_Beta	CEF (SLN)	(1)(1)	(Fe,Mg,Mn,Ni)(Fe,Mn,Ni)
MnSn2	CEF (ST2)	(1)(2)	(Mn)(Sn)
MnZn9	CEF (ST2)	(0.1)(0.9)	(Mn)(Zn)
Ni16Si7Ti6	CEF (SLN)	(16)(7)(6)	(Ni)(Si)(Si,Ti)
Ni2SiZn	CEF (ST3)	(2)(1)(1)	(Ni)(Si)(Zn)
Ni2SiZn3	CEF (ST3)	(2)(1)(3)	(Ni)(Si)(Zn)
Ni2Si_H	CEF (SLN)	(1)(1)(1)	(Ni)(Ni,Va)(Al,Si)
Ni2Si_L	CEF (SLN)	(2)(1)	(Fe,Ni)(Al,Si)
Ni3Si2	CEF (SLN)	(3)(2)	(Fe,Mn,Ni)(Si)
Ni3Si2Zn	CEF (ST3)	(3)(2)(1)	(Ni)(Si)(Zn)
Ni3SiTi2	CEF (SLN)	(3)(1)(2)	(Ni,Si)(Ni,Si)(Ti)
Ni3Si_H	CEF	(3)(1)	(Ni)(Al,Si)

Name	Model	Lattice Size	Constituent
	(SLN)		
Ni3Si_L	CEF (SLN)	(3)(1)	(Ni)(Si,Ti)
Ni3Sn2	CEF (SLN)	(0.5)(0.25) (0.25)	(Ni,Sn)(Ni)(Ni)
Ni3Sn4	CEF (SLN)	(0.4286) (0.5714)	(Ni)(Ni,Sn)
Ni3Sn_H	CEF (SLN)	(0.75)(0.25)	(Ni,Sn)(Ni,Sn)
Ni3Sn_L	CEF (SLN)	(0.75)(0.25)	(Ni,Sn)(Ni,Sn)
Ni3Ti	CEF (SLN)	(0.75)(0.25)	(Fe,Ni,Ti)(Fe,Ni,Si,Ti)
Ni4Si3Ti	CEF (SLN)	(4)(3)(1)	(Ni,Ti)(Si)(Ti)
Ni4Si7Ti4	CEF (SLN)	(4)(7)(4)	(Ni)(Si,Ti)(Si,Ti)
Ni5Si2	CEF (SLN)	(5)(2)	(Fe,Ni)(Al,Si)
Ni5SiTi6	CEF (ST3)	(5)(1)(6)	(Ni)(Si)(Ti)
Ni9Si2Zn	CEF (ST3)	(9)(2)(1)	(Ni)(Si)(Zn)
NiSi	CEF (SLN)	(1)(1)	(Fe,Ni,Zn)(Si)
NiSi4Ti4	CEF	(1)(4)(4)	(Ni)(Si)(Ti)

Name	Model	Lattice Size	Constituent
	(ST3)		
NiSiTi	CEF (SLN)	(1)(1)(1)	(Ni,Ti)(Si)(Ni,Ti)
NiZn8	CEF (ST2)	(0.111) (0.889)	(Ni)(Zn)
NiZn_Beta1	CEF (SLN)	(1)(1)	(Al,Ni,Zn)(Ni,Zn)
NiZn_Gamma	CEF (SLN)	(1)	(Ni,Zn)
Pb12O17	CEF (ST2)	(12)(17)	(Pb)(O)
Pb12O19	CEF (ST2)	(12)(19)	(Pb)(O)
Pb3O4	CEF (ST2)	(3)(4)	(Pb)(O)
PbO_alpha	CEF (ST2)	(1)(1)	(Pb)(O)
PbO_beta	CEF (ST2)	(1)(1)	(Pb)(O)
Phi_Al2Mg5Zn2	CEF (SLN)	(6)(5)	(Mg)(Al,Zn)
Quartz	CEF (ST2)	(1)(2)	(Si)(O)
R3Al11_HT	CEF (ST2)	(11)(3)	(Al)(Ce)
R3Al11_LT	CEF	(11)(3)	(Al)(Ce)

Name	Model	Lattice Size	Constituent
	(ST2)		
R3Al_HT	CEF (ST2)	(1)(3)	(Al)(Ce)
R3Al_LT	CEF (ST2)	(1)(3)	(Al)(Ce)
RAl	CEF (ST2)	(1)(1)	(Al)(Ce)
RAl3	CEF (ST2)	(0.75)(0.25)	(Al)(Ce)
RAl3_HT	CEF (ST2)	(0.75)(0.25)	(Al)(Ce)
Rutile	CEF (SLN)	(1)(2)	(Mn+4,Pb+4,Sn+4,Ti+3,Ti+4)(O-2,Va)
Si2Ti	CEF (SLN)	(0.666667) (0.333333)	(Al,Si)(Ti)
Si4Ti5	CEF (ST2)	(0.444444) (0.555556)	(Si)(Ti)
SiO_AM	CEF (ST2)	(1)(1)	(Si)(O)
SiTi	CEF (SLN)	(0.5)(0.5)	(Al,Si)(Ti)
SiTi3	CEF (ST2)	(0.25)(0.75)	(Si)(Ti)
Sigma	CEF (SLN)	(8)(4)(18)	(Al,Fe,Mn,Ni,Si)(Fe,Si,Ti)(Al,Fe,Mn,Ni,Si,Ti)
Sn3Ti2	CEF	(0.6)(0.4)	(Sn)(Ti)

Name	Model	Lattice Size	Constituent
	(ST2)		
Sn3Ti5	CEF (ST2)	(3)(5)	(Sn)(Ti)
Sn5Ti6	CEF (ST2)	(5)(6)	(Sn)(Ti)
SnTi2	CEF (ST2)	(1)(2)	(Sn)(Ti)
SnTi3	CEF (SLN)	(0.75)(0.25)	(Ti)(Sn,Ti)
Spinel	CEF (SLN)	(1)(2)(2)(4)	(Al+3,Fe+2,Fe+3,Ni+2)(Al+3,Fe+2,Fe+3,Va)(Fe+2,Va)(O-2)
T10_AlFeSi	CEF (ST3)	(0.6)(0.25)(0.15)	(Al)(Fe)(Si)
T11_AlFeSi	CEF (ST3)	(0.6538)(0.2308)(0.1154)	(Al)(Fe)(Si)
T1_AlFeSi	CEF (SLN)	(5)(3)	(Al,Si)(Fe)
T3_AlFeSi	CEF (ST3)	(0.55)(0.25)(0.2)	(Al)(Fe)(Si)
T7_AlFeSi	CEF (SLN)	(0.75)(0.25)	(Al,Si)(Fe)
T8_AlFeSi	CEF (SLN)	(0.66667)(0.33333)	(Al,Si)(Fe)
T_AlMgZn	CEF (SLN)	(26)(6)(48)(1)	(Mg)(Al,Mg)(Al,Mg,Zn)(Al)

Name	Model	Lattice Size	Constituent
T_FeNiZn	CEF (SLN)	(1)(5)	(Fe,Ni,Zn)(Zn)
Ti10O19	CEF (ST2)	(10)(19)	(Ti)(O)
Ti20O39	CEF (ST2)	(20)(39)	(Ti)(O)
Ti2Zn	CEF (ST2)	(2)(1)	(Ti)(Zn)
Ti3O2	CEF (ST2)	(3)(2)	(Ti)(O)
Ti3O5	CEF (ST2)	(3)(5)	(Ti)(O)
Ti3Zn22	CEF (ST2)	(3)(22)	(Ti)(Zn)
Ti4O7	CEF (ST2)	(4)(7)	(Ti)(O)
Ti5O9	CEF (ST2)	(5)(9)	(Ti)(O)
Ti6O11	CEF (ST2)	(6)(11)	(Ti)(O)
Ti7O13	CEF (ST2)	(7)(13)	(Ti)(O)
Ti8O15	CEF (ST2)	(8)(15)	(Ti)(O)
Ti9O17	CEF (ST2)	(9)(17)	(Ti)(O)

Name	Model	Lattice Size	Constituent
TiAlSi_Tau1	CEF (SLN)	(8)(16)	(Al,Ti)(Al,Si)
TiAlSi_Tau2	CEF (SLN)	(1)(2)	(Ti)(Al,Si)
TiOx	CEF (SLN)	(1)(1)(1)	(Ti+2,Ti+3,Va)(Ti,Va)(O-2)
TiZn	CEF (ST2)	(1)(1)	(Ti)(Zn)
TiZn16	CEF (ST2)	(1)(16)	(Ti)(Zn)
TiZn2	CEF (ST2)	(1)(2)	(Ti)(Zn)
TiZn3	CEF (ST2)	(1)(3)	(Ti)(Zn)
Tridymite	CEF (ST2)	(1)(2)	(Si)(O)
X_RE2O3	CEF (SLN)	(2)(2)(1)	(Ce+3,Ce+2)(O-2)(O-2,Va)
ZnO	CEF (ST2)	(1)(1)	(Zn)(O)
a_Ce2Ni7	CEF (ST2)	(0.2222) (0.7778)	(Ce)(Ni)