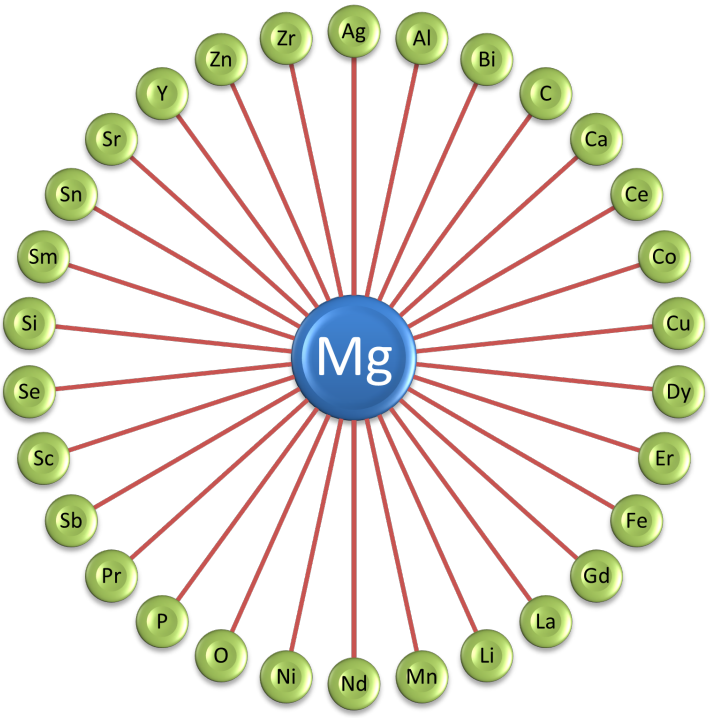
Pandat 2025

Database Manual

CompuTherm LLC

PanMagnesium

Database for multi-component Magnesium-rich casting and wrought alloys



PANDAT™
SOFTWARE

Contents

1 Thermodynamic Database

1.1 Components (31)

Total of **31** components are included in the database as listed here:

Ag-Al-Bi-C-Ca-Ce-Co-Cu-Dy-Er-Fe-Gd-La-Li-**Mg**-Mn-Nd-Ni-O-P-Pr-Sb-Sc-Se-Si-Sm-Sn-Sr-Y-Zn-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 .

Table 1.1: Suggested composition range

Elements	Composition Range (wt.%)
Mg	70 ~ 100
Ag, Al, Ca, Ce, Co, Cu, Er, Fe, Gd, La, Li, Mn, Nd, Ni, Sb, Sc, Si, Sm, Sn, Sr, Y, Zn, Zr	0 ~ 15
Bi, Dy, Pr	0 ~ 2
C, O, P, Se	0 ~ 0.5

There is no composition limit for most binary and many ternary systems formed with major components. These subsystems are valid in the full composition range from 0-100%

as detailed in 1 ~ 1 below. Oxygen containing systems are generally restricted to solid oxides and temperature below 1000°C, only the Mg-Ca-O and Si-O systems include the liquid oxide.

1.3 Phases

Total of **854** phases are included in the database. The phase names are selected according to the following strict rules in Table 1.2 for consistent and intuitive phase identification in different categories. In the category of solid solution phases, indicated in the TDB Viewer of Pandat as CEF(SLN), we distinguish

SE = Solution phase extending to at least one stable phase of an elemental component, disordered.

SI = Solution intermetallic phase usually described by a model with more than one sublattice.

In the category of **stoichiometric** phases (fixed composition) the **TDB Viewer** of Pandat displays **CEF(ST*)**, where * indicates the number of components:

ST1 = Unary stoichiometric phase

ST2 = Binary stoichiometric phase

ST3 = Ternary stoichiometric phase

ST4 = Quaternary stoichiometric phase.

Table 1.2: Rules for phase names in PanMg

Category	Rule for phase name
SE solution CEF(SLN)	Structure names of all solid solution phases stable as **Element**: Bcc, Bct, Cbcc, Cub, Dhcp, Fcc, Hcp, Rhomb, Rhomb_C19, Si_diam. Phase Cub (A13) is stable as βMn.
SI solution	Name = **Selected** approximate chemical stoichiometric formula.

Category	Rule for phase name
CEF(SLN)	• Name is selected close to an important/dominant binary or ternary intermetallic phase with approximate stoichiometry: Al12Mg17, R5Mg41, ... • Name always starts with first element. Elements alphabetical (AlFe, not FeAl). Exceptions: **rare earth** – metal – **non-metal**. • Wild card "elements" R, M, X are used for extended solution ranges: **R** = Rare earth element (La, Ce,..., Lu)*, **M** = metal, **X** = non-metal (C, N, O, F, P, S, Cl, As, Se, Br, Sb, Te, I)**. Examples: RAl, RCu6, RMg, RMg12, Mg2M • Phases may be distinguished/marked by affix for **crystal structure**: MgZn2_C14, MgZn2_C36, ..., AlCaMg_C36, R8Mg70Zn6_14H • Phase name may be **crystal prototype name**, such as CaCu5; that phase is stable as binary CaCu5, CeCu5, Cu5Gd, LaCu5, Cu5Nd, CaNi5,CeNi5, LaNi5, GdNi5, and NdNi5. • Temperature **polymorphs** may be distinguished by affix _T1 (low temperature), _T2, _T3 (high temperature). • **Well established phase names** might be given as affix, RM3_W, YZn5_H, ..., AlMgZn_phi, AlMgZn_tau, AlCu_eps
Stoichiometric CEF(ST1),	Name = **Chemical stoichiometric formula**. • Name always starts with first element. Elements generally

Category	Rule for phase name
CEF(ST2), CEF(ST3), CEF(ST4)	alphabetical; Exceptions: rare earth element (La, Ce, ... Lu) FIRST; non-metal (C, O,) LAST. Examples: AgCa, **Ce**Ag, MgSc, Si**C**, Si3**N**4, Al4Si**C**4, Y2**O**3 **Well established phase names** might be given as affix, upper case: Mg58Y8Zn6_18R, Mg46Y8Zn6_10H Stable **elements** (ST1) are C_graph, Se_A8, and P_ red (P_ white is metastable).

*) Rare earth elements do not include Sc and Y; Lanthanides only R = (La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er,Tm, Yb, Lu).
**) Non-metals are from "Pettifor-string", chemical order from 88 to 102, (Sb, As, P, Te, Se, S, C, I, Br, Cl, N, O, F), and listed according to the periodic table.

The total **854** phases assessed in PanMg2025 comprise the **237** solution phases (gas phase, liquid, plus 235 solid solution phases) and **617** stoichiometric phases. These **617** comprise **4** unary, **519** binary, **92** ternary, and **2** quaternary assessed stoichiometric phases.

As an illustration of the names and models assigned to the various solution and stoichiometric phases a small representative selection is listed in Table 1.3. For all phases assessed in PanMg2025 is listed in PanMg2025:List of All Phases. Users can also view them in the TDB viewer of Pandat software.

Table 1.3: Example of phase names and related information

Name	Model	Lattice Size	Constituent
Liquid	CEF (SLN)	(1)	(Ag,Al,Al2La,Bi,Bi2Mg3,C,Ca,Ca2Sn,CaO, Ce,Co,Cu,Dy,Er,Fe,Gd,La,LaSn,Li, Li2C2,Li4Sn,Mg,Mg2Sn,MgO,Mn, O,P,Nd,Ni,Pr,Sb,Sc,Se,Si, Sm,Sn,Sr,Y,Zn,Zr)
Hcp	CEF (SLN)	(1)(0.5)	(Ag,Al,Bi,Ca,Ce,Co,Cu,Dy,Er,Fe,Gd,La,Li,Mg, Mn,Nd,Ni,O,Pr,Sb,Sc,Se,Si,Sm,Sn,Sr,Y,Zn,Zr) (Va)
Al12Mg17	CEF (SLN)	(10)(24)(24)	(Mg)(Al,Ca,Cu,Li,Mg,Zn)(Al,Cu,Mg,Zn)
Al11Mn4_T1	CEF (SLN)	(11)(4)	(Al)(Fe,Mn)
Al11Mn4_T2	CEF (SLN)	(29)(10)	(Al,Mn)(Mn)
Al2Ca_C15	CEF (SLN)	(0.666667) (0.333333)	(Al,Mg)(Ca,Sr)
CaCu5	CEF (SLN)	(0.166667) (0.833333)	(Ca,Ce,La,Gd,Nd,Y)(Al,Cu,Ni)
CaMgO_ halite	CEF (SLN)	(1)(1)	(Ca,Mg)(O)
Gas	GAS	(1)	(Ag,Al,Al2,Bi,Bi2,C,C2,C3,C4,C5, Ca,Ce,Co,Cu,Cu2,Dy,Er,Fe,Gd,La, Li,Li2,Mg,Mg2,Mn,Nd,Ni,P,P2,P4, Pr,Sb,Sb2,Sc,Sc2,Se,Se2,Se3,Se4, Se5,Se6,Se7,Se8,Si,Si2,Si3,Si4, Sm,Sn,Sr,Y,Zn,Zr,AlC,CSi, CSi2,C2Si,Li3C,Li4C,Li6C,O,O2,O3, Al2O,Al2O2,Al2O3,AlO,AlO2,C2O,C3O2,

Name	Model	Lattice Size	Constituent
			C1O1,C1O2,CaO,CeO,CuO,FeO,La2O, La2O2,LaO,Li2O,Li2O2,LiO,MgO,NdO, NdO2,NiO,PrO,ScO,SeO,SeO2,SiO,SiO2, Sn2O2,Sn3O3,Sn4O4,SnO,SnO2,Sr2O, SrO,YO,ZrO,ZrO2)
GdMg2_ C15L	CEF (SLN)	(0.333333) (0.666667)	(Gd,Mg,Y)(Gd,Li,Mg,Zn)
RZn2	CEF (SLN)	(0.333333) (0.666667)	(Ce,Gd,La,Nd)(Zn)
R5Mg41	CEF (SLN)	(5)(41)	(Ca,Ce,La,Nd,Pr,Y)(Mg,Zn)
Si_diam	CEF (SLN)	(1)	(Al,C,Li,Mg,Mn,O,P,Sb,Si,Sn,Zn)
Ag2Ca	CEF (ST2)	(0.666667) (0.333333)	(Ag)(Ca)

**For liquidus projection calculations it is usually recommended to suspend the gas phase*

1.4 What is new in PanMg2025

Following the last grand revision and upgrade made with **PanMg2024** the quality and scope of thermodynamic data and phase diagrams have been continuously improved and expanded for **PanMg2025**.

Key improvements include:

- 6 new or improved binary system descriptions of Al-La, Ce-Sn, Fe-Mg, Gd-La, La-Y, Mg-Nd.

- 20 new or improved ternary system descriptions of Ag-Gd-Mg, Ag-La-Mg, Al-Ce-La, Al-Gd-La, Al-Gd-Mg, Al-La-Mg, Al-La-Nd, Al-La-Y, Al-Li-Mg, Ca-Mg-Zn, Ce-La-Mg, Ce-Mg-Zn, Cu-Mg-Y, Gd-La-Mg, Gd-Mg-Mn, La-Mg-Nd, Mg-Mn-Y, Mg-Nd-Y, Mg-Nd-Zn, Mg-Y-Zr.

1.5 Assessed Subsystems

A total of **384** systems, including 250 binary, 117 ternary and 17 quaternary 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 (250)

Ag-Al(10)	Ag-Ca(10)	Ag-Ce(10)	Ag-Co(10)	Ag-Cu(10)	Ag-Er(10)	Ag-Fe(10)
Ag-Gd(10)	Ag-La(10)	Ag-Mg(10)	Ag-Mn(10)	Ag-Nd(5)	Ag-Ni(10)	Ag-Sb(10)
Ag-Sc(10)	Ag-Si(10)	Ag-Sm(10)	Ag-Sn(5)	Ag-Sr(10)	Ag-Y(5)	Ag-Zn(10)
Ag-Zr(5)	Al-Bi(10)	Al-C(10)	Al-Ca(10)	Al-Ce(10)	Al-Co(10)	Al-Cu(10)
Al-Er(10)	Al-Fe(10)	Al-Gd(10)	Al-La(10)	Al-Li(10)	Al-Mg(10)	Al-Mn(10)
Al-Nd(10)	Al-Ni(10)	Al-P(10)	Al-Pr(10)	Al-Sb(10)	Al-Sc(10)	Al-Si(10)
Al-Sm(10)	Al-Sn(10)	Al-Sr(10)	Al-Y(10)	Al-Zn(10)	Al-Zr(10)	Bi-Mg(10)
Bi-O(5)	Bi-Sb(10)	Bi-Sn(10)	Bi-Zn(10)	C-Ca(5)	C-Li(10)	C-Mg(10)
C-Si(10)	C-Sn(10)	Ca-Ce(5)	Ca-Cu(10)	Ca-Fe(10)	Ca-Gd(5)	Ca-Li(10)
Ca-Mg(10)	Ca-Mn(10)	Ca-Nd(5)	Ca-Ni(5)	Ca-O(10)	Ca-P(5)	Ca-Sb(10)
Ca-Sc(10)	Ca-Si(10)	Ca-Sn(10)	Ca-Sr(10)	Ca-Y(5)	Ca-Zn(10)	Ca-Zr(5)
Ce-Co(10)	Ce-Cu(10)	Ce-Fe(10)	Ce-La(10)	Ce-Li(5)	Ce-Mg(10)	Ce-Mn(5)
Ce-Nd(10)	Ce-Ni(10)	Ce-Sb(10)	Ce-Sc(5)	Ce-Si(5)	Ce-Sn(10)	Ce-Sr(5)
Ce-Y(10)	Ce-Zn(10)	Ce-Zr(5)	Co-Cu(10)	Co-Er(10)	Co-Fe(5)	Co-Gd(10)
Co-La(10)	Co-Mg(10)	Co-Mn(10)	Co-Nd(10)	Co-Ni(10)	Co-Pr(10)	Co-Sb(10)
Co-Sc(5)	Co-Si(10)	Co-Sm(10)	Co-Sn(10)	Co-Y(10)	Co-Zn(10)	Co-Zr(10)
Cu-Er(10)	Cu-Fe(10)	Cu-Gd(10)	Cu-La(10)	Cu-Li(5)	Cu-Mg(10)	Cu-Mn(10)
Cu-Nd(10)	Cu-Ni(10)	Cu-Sb(10)	Cu-Sc(5)	Cu-Si(10)	Cu-Sm(10)	Cu-Sn(10)

Cu-Sr(10)	Cu-Y(10)	Cu-Zn(10)	Cu-Zr(10)	Dy-Mg(10)	Er-Fe(10)	Er-Mg(10)
Er-Sb(10)	Er-Sc(10)	Er-Si(10)	Er-Y(10)	Er-Zn(10)	Fe-Gd(10)	Fe-Mg(10)
Fe-Mn(10)	Fe-Nd(10)	Fe-Ni(10)	Fe-Sb(10)	Fe-Sc(10)	Fe-Si(10)	Fe-Sm(10)
Fe-Sn(10)	Fe-Sr(10)	Fe-Y(10)	Fe-Zn(10)	Fe-Zr(10)	Gd-La(5)	Gd-Li(10)
Gd-Mg(10)	Gd-Mn(10)	Gd-Ni(10)	Gd-Sb(10)	Gd-Sc(5)	Gd-Si(10)	Gd-Sm(10)
Gd-Y(10)	Gd-Zn(10)	Gd-Zr(10)	La-Mg(10)	La-Mn(10)	La-Nd(10)	La-Ni(10)
La-Sb(10)	La-Sc(5)	La-Si(10)	La-Sn(10)	La-Y(10)	La-Zn(10)	Li-Mg(10)
Li-Mn(5)	Li-Sc(10)	Li-Si(10)	Li-Sn(10)	Li-Sr(5)	Li-Y(5)	Li-Zn(5)
Li-Zr(5)	Mg-Mn(10)	Mg-Nd(10)	Mg-Ni(10)	Mg-O(10)	Mg-P(5)	Mg-Pr(10)
Mg-Sb(10)	Mg-Sc(10)	Mg-Se(5)	Mg-Si(10)	Mg-Sm(10)	Mg-Sn(10)	Mg-Sr(10)
Mg-Y(10)	Mg-Zn(10)	Mg-Zr(10)	Mn-Nd(5)	Mn-Ni(5)	Mn-Sc(10)	Mn-Si(10)
Mn-Sm(10)	Mn-Sn(10)	Mn-Sr(10)	Mn-Y(10)	Mn-Zn(10)	Mn-Zr(10)	Nd-Ni(10)
Nd-Y(10)	Nd-Zn(10)	Ni-Sb(10)	Ni-Sc(10)	Ni-Si(10)	Ni-Sm(10)	Ni-Sn(10)
Ni-Sr(10)	Ni-Y(10)	Ni-Zn(10)	Ni-Zr(10)	O-Si(10)	P-Si(10)	Pr-Sb(10)
Sb-Si(10)	Sb-Sm(10)	Sb-Sn(10)	Sb-Zn(10)	Sc-Si(10)	Sc-Sn(10)	Sc-Sr(10)
Sc-Y(10)	Sc-Zn(10)	Sc-Zr(10)	Si-Sn(10)	Si-Sr(10)	Si-Y(5)	Si-Zn(5)
Si-Zr(10)	Sm-Sn(10)	Sm-Zn(10)	Sn-Sr(10)	Sn-Y(10)	Sn-Zn(10)	Sn-Zr(5)
Sr-Y(5)	Sr-Zn(10)	Y-Zn(10)	Y-Zr(10)	Zn-Zr(10)		

Ternary Systems (117)

Ag-Al-Cu(10)	Ag-Al-Mg(5)	Ag-Cu-Mg(5)	Ag-Gd-Mg(10)	Ag-La-Mg(10)	Ag-Mg-Nd(10)
Ag-Mg-Sb(5)	Al-Bi-Mg(10)	Al-C-Mg(10)	Al-C-Si(10)	Al-Ca-Ce(5)	Al-Ca-Fe(5)
Al-Ca-Li(5)	Al-Ca-Mg(10)	Al-Ca-Si(5)	Al-Ca-Sr(10)	Al-Ce-Gd(5)	Al-Ce-La(5)
Al-Ce-Mg(10)	Al-Ce-Mn(5)	Al-Ce-Nd(5)	Al-Ce-Si(10)	Al-Ce-Y(5)	Al-Cu-Gd(5)
Al-Cu-Li(10)	Al-Cu-Mg(10)	Al-Cu-Mn(10)	Al-Cu-Nd(5)	Al-Cu-Si(10)	Al-Cu-Sn(10)
Al-Cu-Zn(10)	Al-Fe-Mn(10)	Al-Fe-Si(10)	Al-Gd-La(5)	Al-Gd-Mg(10)	Al-Gd-Mn(5)
Al-Gd-Nd(5)	Al-Gd-Y(5)	Al-La-Mg(10)	Al-La-Nd(5)	Al-La-Y(5)	Al-Li-Mg(10)
Al-Li-Mn(5)	Al-Li-Si(10)	Al-Mg-Mn(10)	Al-Mg-Sc(10)	Al-Mg-Si(10)	Al-Mg-Sn(10)
Al-Mg-Sr(10)	Al-Mg-Y(5)	Al-Mg-Zn(10)	Al-Mn-Nd(5)	Al-Mn-Sc(5)	Al-Mn-Si(10)

Al-Nd-Y(5)	Al-Si-Y(5)	Al-Si-Zn(5)	Al-Sn-Zn(10)	Bi-Mg-Sn(10)	C-Li-Si(10)
C-Li-Sn(5)	Ca-Ce-Mg(10)	Ca-Fe-Si(10)	Ca-Li-Mg(10)	Ca-Li-Si(10)	Ca-Mg-O(10)
Ca-Mg-Si(10)	Ca-Mg-Sn(10)	Ca-Mg-Sr(10)	Ca-Mg-Zn(10)	Ca-Sr-Zn(5)	Ce-La-Mg(10)
Ce-Li-Mn(5)	Ce-Mg-Mn(5)	Ce-Mg-Nd(10)	Ce-Mg-Sn(10)	Ce-Mg-Y(10)	Ce-Mg-Zn(10)
Cu-Fe-Si(10)	Cu-La-Ni(10)	Cu-Li-Mg(10)	Cu-Mg-Ni (10)	Cu-Mg-Si(10)	Cu-Mg-Y(10)
Cu-Mg-Zn(10)	Cu-Ni-Si(5)	Cu-Sn-Zn (5)	Cu-Y-Zr(10)	Fe-Mg-Si (10)	Fe-Mn-Si(10)
Gd-La-Mg(5)	Gd-Li-Mg(10)	Gd-Mg-Mn(10)	Gd-Mg-Y(10)	Gd-Mg-Zn(10)	La-Mg-Nd(10)
La-Mg-Si(5)	La-Mg-Zn(10)	Li-Mg-Mn(5)	Li-Mg-Si(10)	Li-Mg-Zn(10)	Li-Si-Sn(5)
Mg-Mn-Sc(5)	Mg-Mn-Si(5)	Mg-Mn-Sr(10)	Mg-Mn-Y(10)	Mg-Mn-Zn(10)	Mg-Mn-Zr(5)
Mg-Nd-Y(10)	Mg-Nd-Zn(10)	Mg-Ni-Si(5)	Mg-Si-Sn(10)	Mg-Si-Zn(5)	Mg-Sn-Zn(10)
Mg-Y-Zn(10)	Mg-Y-Zr(5)	Mn-Y-Zr(10)			

Quaternary Systems (17)

Ag-Al-Cu-Mg(5)	Al-Bi-Mg-Sn(10)	Al-Ca-Ce-Mg(5)	Al-Ca-Li-Mg(5)	Al-Ca-Mg-Mn(9)
Al-Ce-Li-Mg(5)	Al-Cu-Mg-Si(10)	Al-Cu-Mg-Zn(10)	Al-Li-Mg-Si(10)	Al-Mg-Mn-Zn(10)
Ca-Ce-Mg-Sn(10)	Ca-Mg-Si-Sn (10)	Ce-Gd-Mg-Y(5)	Gd-Mg-Mn-Sc(5)	Gd-Mg-Y-Zn(9)
Mg-Mn-Sc-Y(5)	Mg-Mn-Y-Zr(5)			

1.6 Database Validation

The early development of the Mg-database, starting in 1995, is described in [2001Sch] and aspects of quality assurance were first given by [2005Sch].

Progress in systematic development and applications of the current thermodynamic database for Mg alloys is reported in detail in [2018Sch] and [2019Sch]. Models for multicomponent alloys are built in a methodical approach from quantitative descriptions of unary, binary and ternary subsystems [2012Sch]. For a large number of ternary- and some higher- alloy systems, an evaluation of the modeling depth is made with concise reference to experimental work validating these thermodynamic descriptions. A special focus is on ternary intermetallic phase compositions. These comprise solutions of the third component in a binary compound as well as truly ternary solid solution phases, in addition to the simple

ternary stoichiometric phases. Concise information on the stability ranges is given. That evaluation is extended to selected quaternary and even higher alloy systems. Thermodynamic descriptions of intermetallic solution phases guided by their crystal structure are also elaborated and the diversity of such unified phases is emphasized [2012Sch].

Key issues in this large thermodynamic Mg alloy database are consistency, coherency and quality assurance. These issues and the basic concept are elaborated in [2013Gro]. The structurally supported modeling, especially of pertinent solid phases, requires proper consideration of multicomponent solid solutions of intermetallic phases which are abundant in magnesium alloys. Moreover, evidence on the database application by predicting phase formation during solidification or heat treatment in advanced multicomponent magnesium alloys from thermodynamic calculations is given in detail in [2013Gro]. Highlights of the most recent progress are given in [2015Sch1].

The growing modeling depth of the PanMagnesium database enhances predictive type calculations of phase formation during solidification, heat treatment or other processing steps of Mg alloys. Evidence is given by comparing the results of such calculations with the phase formation reported in studies of advanced magnesium alloys, such as Mg-Zn-Y/Zr/Gd/Ce/Nd, Mg-Al-Ca/Mn/Sr/Sn, Mg-Sn-Ca and higher order Mg-Al-Sn-Ca/Sr and Mg-Sn-Ca-Ce/Gd/Zr alloys [2013Gro]. Reference is made to the extensive material provided in that most current publication which is not repeated here.

The current thermodynamic database for magnesium alloys has also been extensively tested and validated using published experimental data [1998Lia, 1999Gro, 2001Gro4, 2001Gro6, 2001Kev1, 2001Kev2, 2001Kev3, 2002Gro1, 2002Gro2, 2003Gro1, 2003Gro2, 2004Bru, 2004Kev, 2004Gro, 2006Ohn4]. Some sub-quaternary systems of this database have been critically assessed: Mg-Al-Ca-Ce, Mg-Al-Ca-Li, Mg-Al-Ce-Li, Mg-Al-Cu-Zn, Mg-Mn-Y-Zr. The quaternary systems Mg-Al-Li-Si [2001Kev4] and Mg-Ce-Mn-Sc, Mg-Gd-Mn-Sc, Mg-Mn-Sc-Y [2000Pis2, 2001Gro2] were thermodynamically modeled and used for technical applications.

For the reliability of the calculated phase diagrams the fitting of the invariant temperatures are of paramount importance. Since the measured temperatures of the invariant reactions are not affected by super-cooling related problems, these nonvariant data are perfect criteria for comparison of experimental with calculated data (as shown in Figure 1.1).

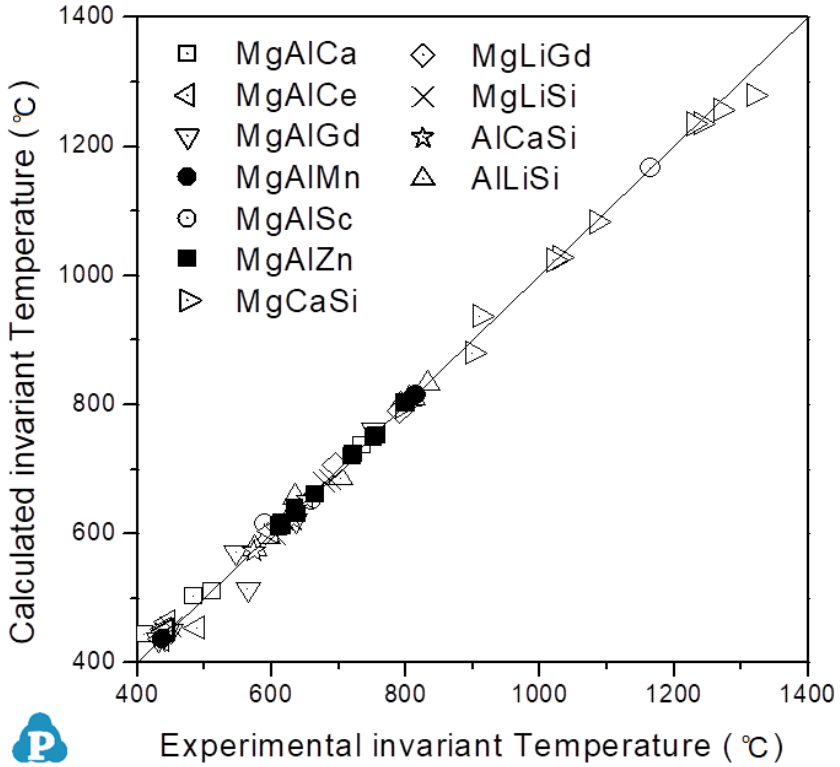


Figure 1.1: Invariant temperatures for various ternary alloys included in PanMagnesium: Comparison between calculated and experimental data

For the Mg-Al-Mn system the reliability is checked in detail [2005Ohn]. The liquidus surface of the Mg-rich corner is shown in Figure 1.2. The same experimental data are plotted in Figure 1.3 as comparison between calculated results and experimental data.

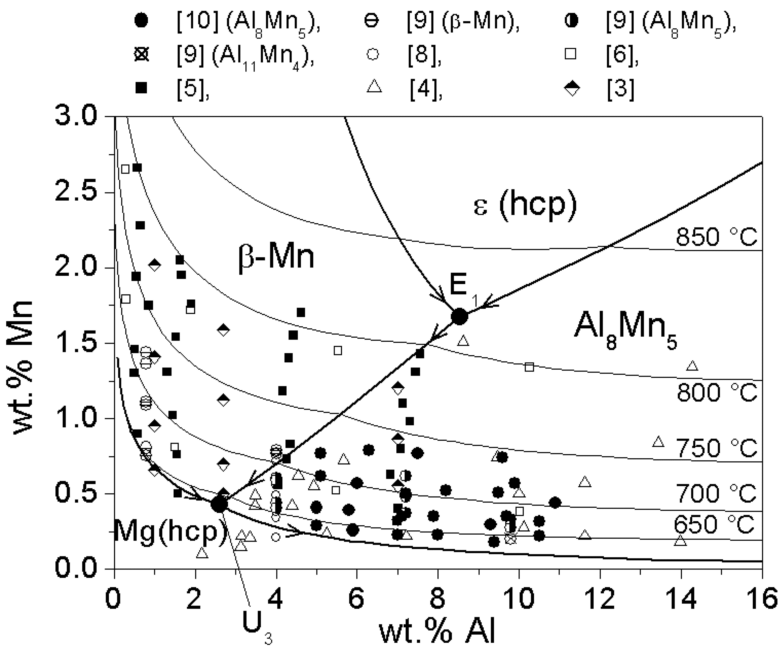


Figure 1.2: Calculated partial liquidus surface, the thick lines indicate monovariant reaction lines and the thin lines represents the isotherms. Superimposed are the compositions of experimental alloys further compared to calculated data of the liquidus surface. The primary solid phase is specified in some experimental data

This comparison in Figure 1.3 enables easy identification of those groups of experimental data that are not consistent with the bulk of experimental work. There is a reasonable agreement with this bulk of experimental data and the calculated values. Moreover, there is a reasonable agreement with the primary solidifying phases as shown in Figure 1.2.

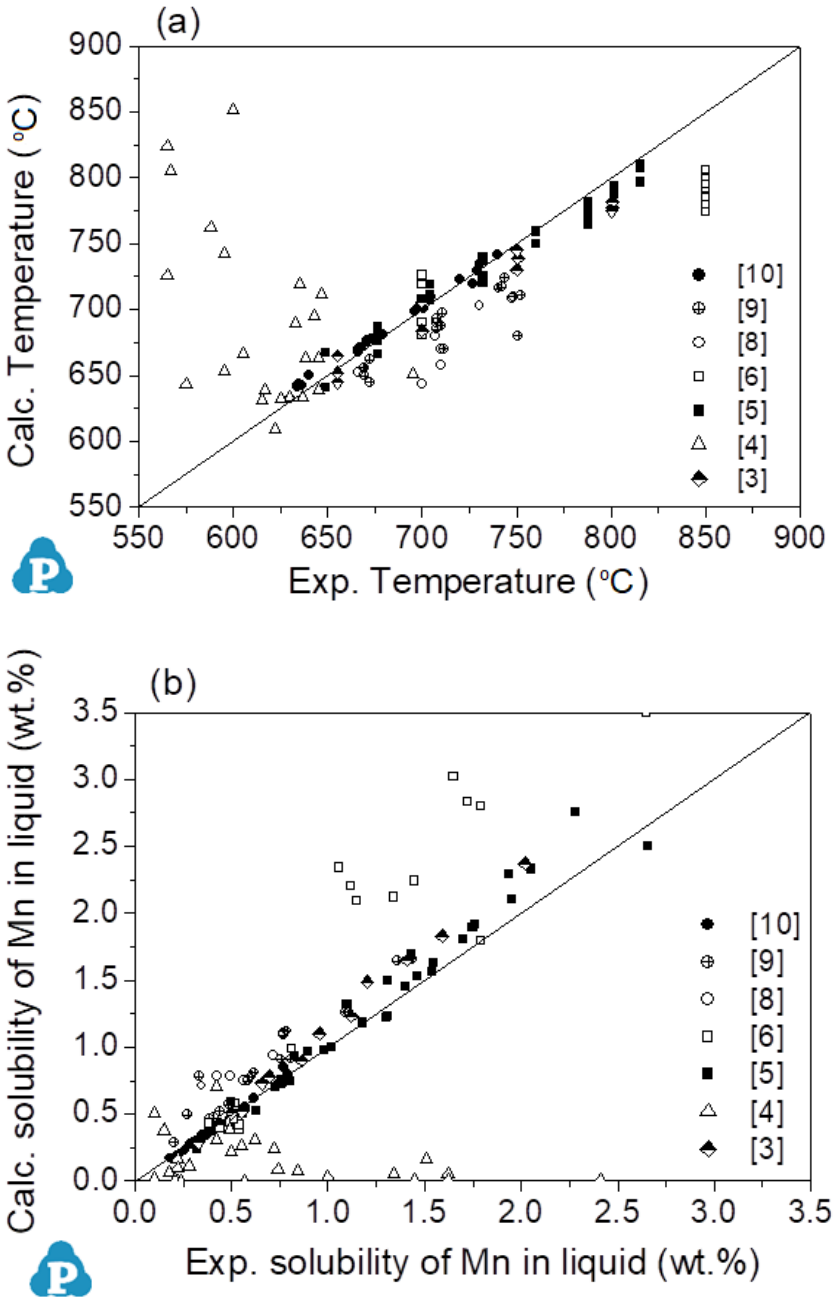


Figure 1.3: Comparison between calculated results and experimental data for all alloy samples in the Mg-Al-Mn system. (a) Liquidus temperature at a given composition, (b) Solubility of Mn in liquid at a given temperature and Al composition. The straight line in Figs. (a) and (b) is a visual aid corresponding to perfect agreement between experimental values and the calculated results from the present thermodynamic model

The experimental data for the commercially very important Mg-Al-Zn alloys are shown in Figure 1.4 [2006Ohn1]. The liquidus surface of the Mg-rich corner is given inFigure 1.4. The same experimental data is plotted in Figure 1.5 as comparison between calculated results and experimental data. A similar comparison was done for the Mg-rich phase equilibria of the Mg-Mn-Zn system [2006Ohn2]. Technical important liquidus and Solidus temperatures of Mg-rich Mg-Al-Mn-Zn Alloys (AZ series) were investigated by [2006Ohn3].

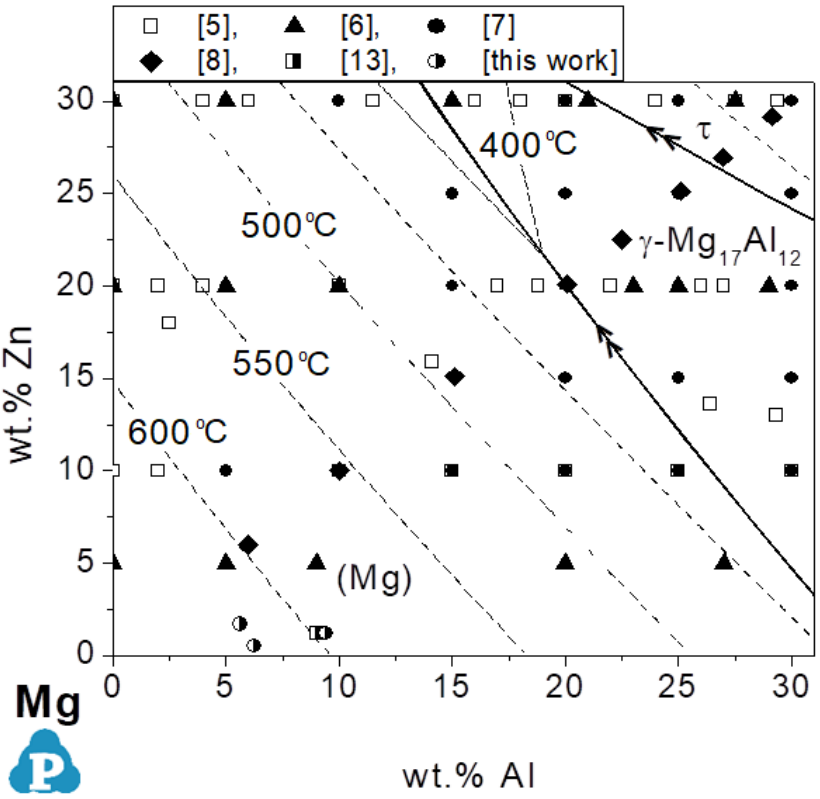


Figure 1.4: Calculated partial Mg-Al-Zn liquidus surface and experimental alloy compositions. The thick lines indicate monovariant reaction lines and the dashed lines represent isotherms at an interval of 50°C

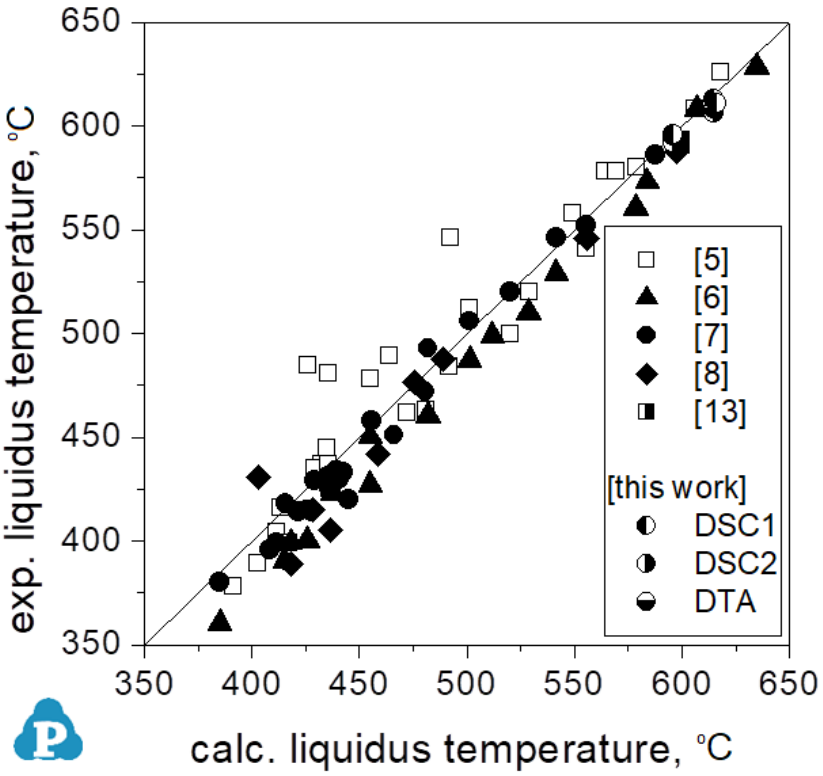


Figure 1.5: Comparison between calculated and experimental liquidus temperature for all alloy samples in the Mg-Al-Zn system. The straight line is a visual aid corresponding to perfect agreement between experimental and calculated results

Measured liquidus temperatures for other ternary Mg-alloy systems are compared in Figure 1.6 with calculations from the magnesium database. These miscellaneous Mg-X1-X2 systems include the alloying elements Al, Ca, Ce, Gd, Li, Sc, and Si.

Additionally, a selected comparison of experimental data and calculated phase equilibria is given below. This demonstrates the feasibility to perform reasonable calculations with PanMagnesium even in some very high alloyed regions with vanishing Mg-content as outlined in Figure 1.6. For the Al-Li-Si system a comparison between calculated and experimentally measured DTA data is given in Figure 1.7 [2001Gro6]. Figure 1.8 shows a calculated vertical section in the Al-Ce-Si system at constant 90at% Al including the DSC/DTA signals measured [2004Gro].

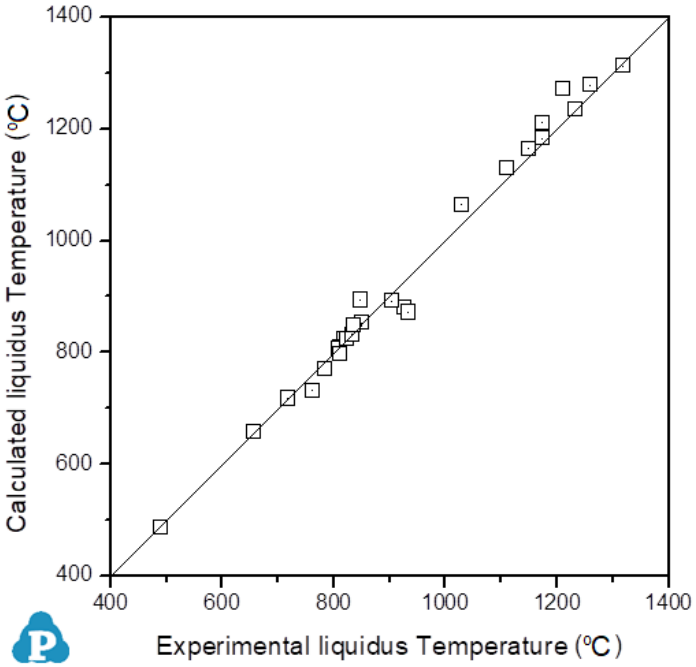


Figure 1.6: Liquidus temperatures for various ternary magnesium alloys outside the Mg-Al-Mn-Zn system, with alloying elements Al, Ca, Ce, Gd, Li, Sc, Si: Comparison between calculated and experimental data

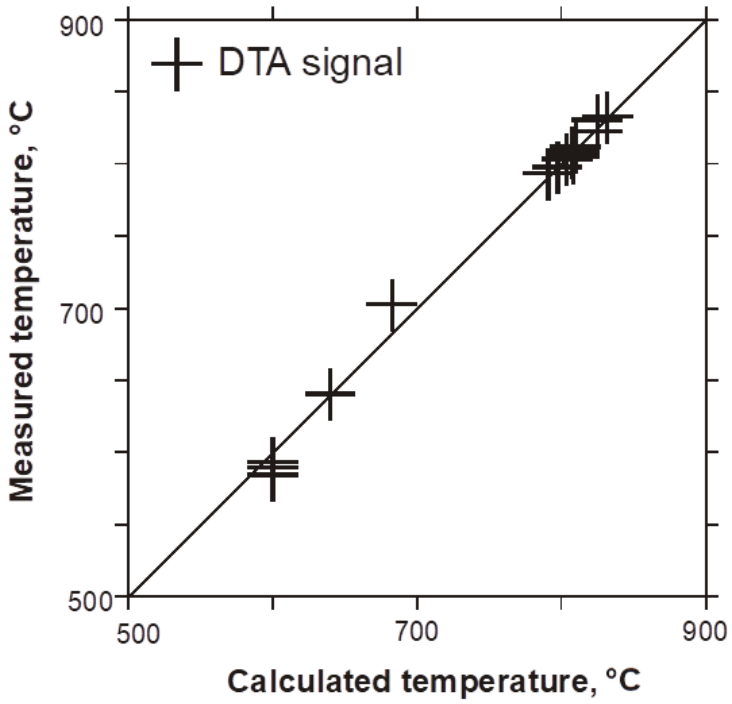


Figure 1.7: Comparison between calculated and experimentally measured DTA data for the Al-Li-Si system

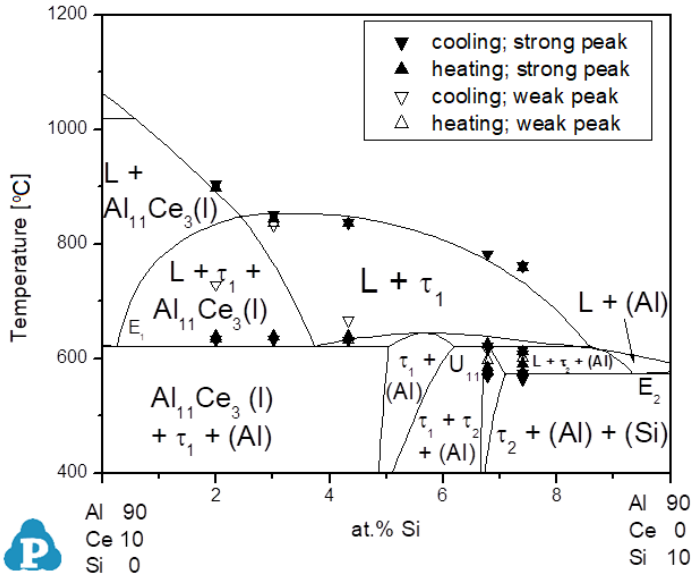


Figure 1.8: Calculated vertical section Al90Ce10 - Al90Si10 at constant 90at%Al including the DSC/DTA signals measured in [2004Gro]

Advanced Mg alloys employing Long Period Stacking Order (LPSO) and icosahedral precipitate phases for superior properties have been studied in more depth recently. For the most important ternary alloy systems Mg-Y-Zn and Mg-Gd-Zn, these findings are used to advance the description in PanMg beyond the previous knowledge [2015Sch2, 2015Gro].

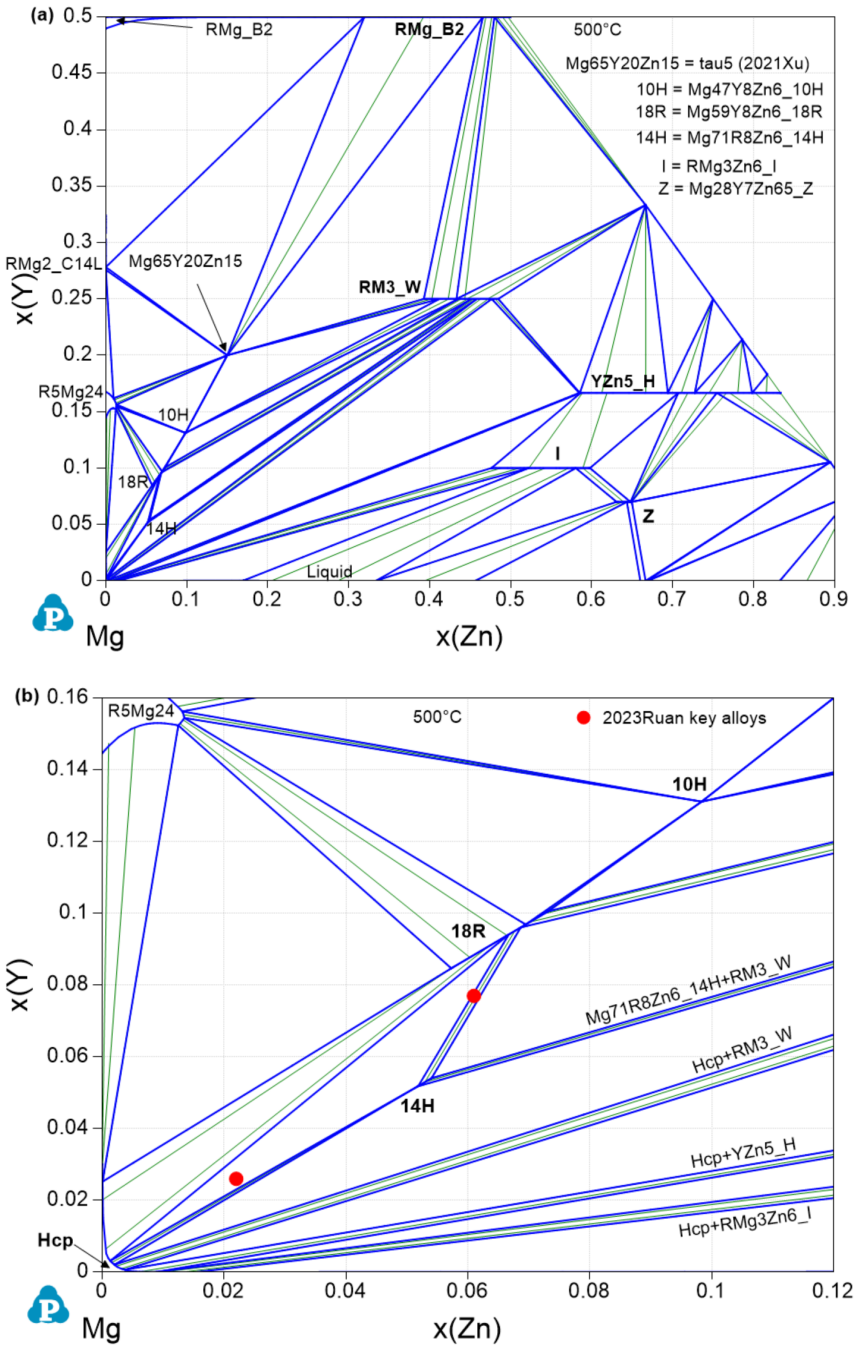


Figure 1.9: Calculated Mg-Y-Zn isothermal section at 500°C; (a) up to 50 at.% Y and 90 at.% Zn; (b) up to 16 at.% Y and 12 at.% Zn compared with the key alloys of [2023Rua]

That is exemplified for Mg-Y-Zn in the calculated isothermal sections at 500°C shown for Mg-rich corner in Figure 1.9. The detail in Figure 1.9b shows the perfect agreement with the dedicated TEM study of the two key alloys of [2023Rua] in the 14H+18R two-phase and (Mg)+14H+18R three-phase regions. This also reflects the experimentally verified solid solution ranges of these two LPSO phases 14H and 18R in the TEM studies [2021Rua1, 2021Rua2], confirmed by the experimental data indicated in [2015Sch2], that were simplified to stoichiometric phases at that time in PanMg2015 and the previous study [2012Gro]. The phase equilibria at lower Mg-content in Figure 1.9a are also confirmed by the mutually consistent experimental data assessed from [2012Gro, 2015Sch2, 2021Xu1] and include the new compound Mg65Y10Zn15 [2021Xu1].

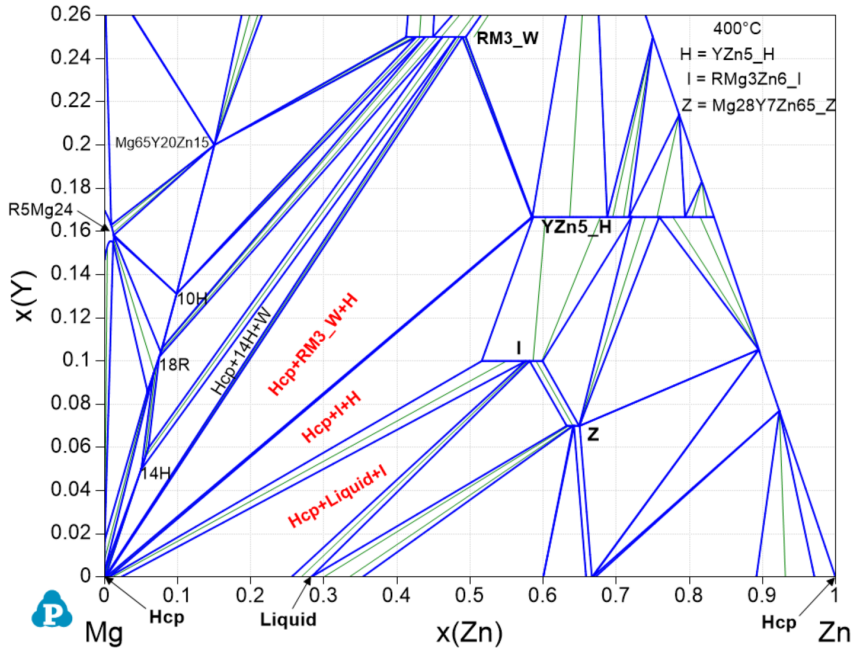


Figure 1.10: Calculated Mg-Y-Zn isothermal section at 400°C up to 26 at.% Y and 100 at.% Zn; three-phase regions (Mg)+Liquid+I, (Mg)+I+H, and (Mg)+RM3_W verified by the key alloys of [2020Liu] are marked red.

At 400°C the equilibria (Mg)+Liquid+I, as opposed to (Mg)+Liquid+Z, as well as (Mg)+I+H and (Mg)+RM3_W, confirmed by TEM [2020Liu], are exactly represented in the Mg-Y-Zn isothermal section of Figure 1.10 calculated with PanMg2025. None of the currently

published alternative CALPHAD descriptions, e.g. [2021Xu1, 2023Rua], is capable of describing the entity of experimentally verified data of the Mg-Y-Zn system as shown by PanMg2025.

The Mg-Gd-Zn system includes the solid-solution LPSO phase 14H and the re-optimization is validated by the experimental data of the entire stable phase equilibria [2012Qi, 2015Gro] as well as the intricate metastable phases I and H2 [2016Gro]. The experimental fact that after heat treatment at 400 or 500°C, the I and the H2 phases, observed in cast alloys, transform into the stable phases F and H1 [2016Gro] are reflected in the Mg-Gd-Zn isothermal sections at 400 and 500°C for the stable system and the metastable system with suspended phases F and H1, calculated with PanMg2024. In addition, the more recent experimental data [2023Xu, 2021Xu2, 2021Liu] were considered but found less conclusive. The as-cast formation conditions of the icosahedral I phase, modeled as RMg3Zn6_I with R = (Y,Gd) solubility, is detailed in the calculated Mg-Gd-Zn liquidus projections for the stable system, Figure 1.11, and the metastable system, Figure 1.12, where only a small supercooling leads to the crystallization fields of I and H2 phases. These data are, in addition to [2016Gro], validated by the experimental studies of as-cast [2008Liu, 2014Sri, 2016Li, 2018Luo] and directionally solidified [2017Yan] alloys. As example, the Scheil-simulated solidification paths superimposed on Figure 1.12 for the two alloys with high Zn/Gd ratio [2014Sri#2, 2008Liu] demonstrate after primary (Mg) the secondary phases RM3_W and RMg3Zn6_I as also observed experimentally. By contrast, the alloy with low Zn/Gd ratio [2014Sri#3] show after primary (Mg) only the secondary phase RMg3 (with 23 at.% Zn) at the Scheil-solidus of 555°C. For that alloy the equilibrium calculation indicates the formation of 14H in the reaction RMg3 + (Mg) = 14H at about 536°C. That is well verified by the observed microstructure where the small fraction of LPSO phase next to RMg3 in alloy #3 was assumed to be formed due to the relatively slow cooling rate [2014Sri].

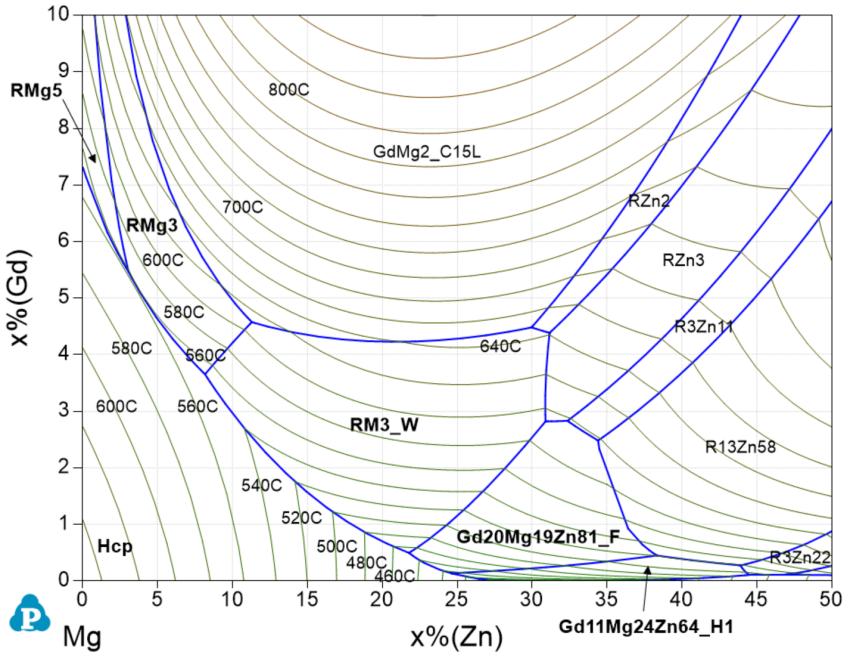


Figure 1.11: Calculated Mg-Gd-Zn liquidus projection up to 10 at.% Gd and 50 at.% Zn include the stable phases F and H1.

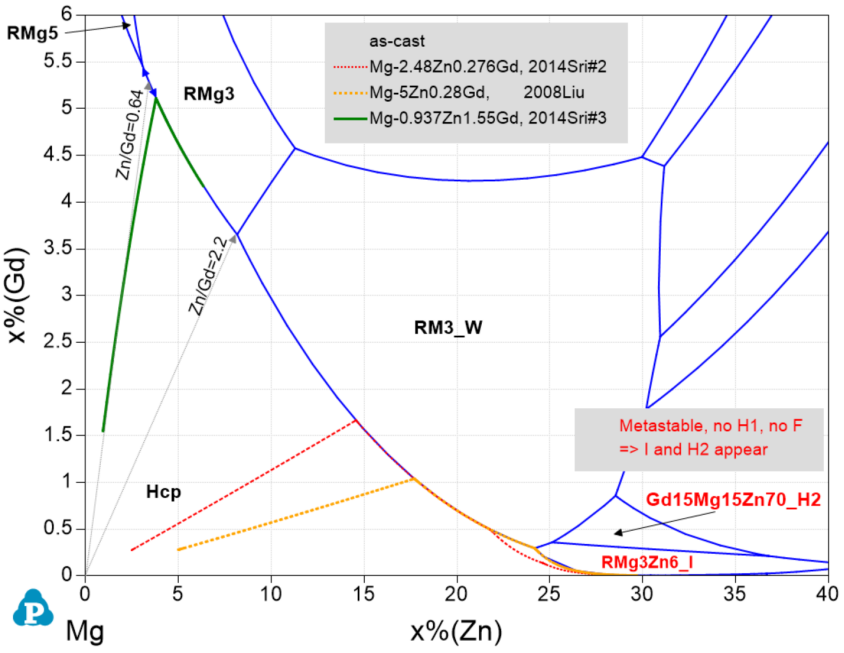


Figure 1.12: Calculated Mg-Gd-Zn metastable liquidus projection up to 6 at.% Gd and 40 at.% Zn with phases F and H1 suspended, thus, the next stable phases I and H2 appear. Scheil-simulated solidification paths of three alloys are superimposed, see text.

Another highlight of PanMg is the incorporation of oxygen as an element and all relevant solid oxides and gas species. For example, the reaction of Mg with CaO during melting and solidification was studied experimentally and the thermodynamic description of the Mg-Ca-O system was developed with scrutinized oxide data. The calculated isothermal section in Figure 1.13 is also validated using in-situ synchrotron radiation diffraction [2018Lia1, 2018Lia2].

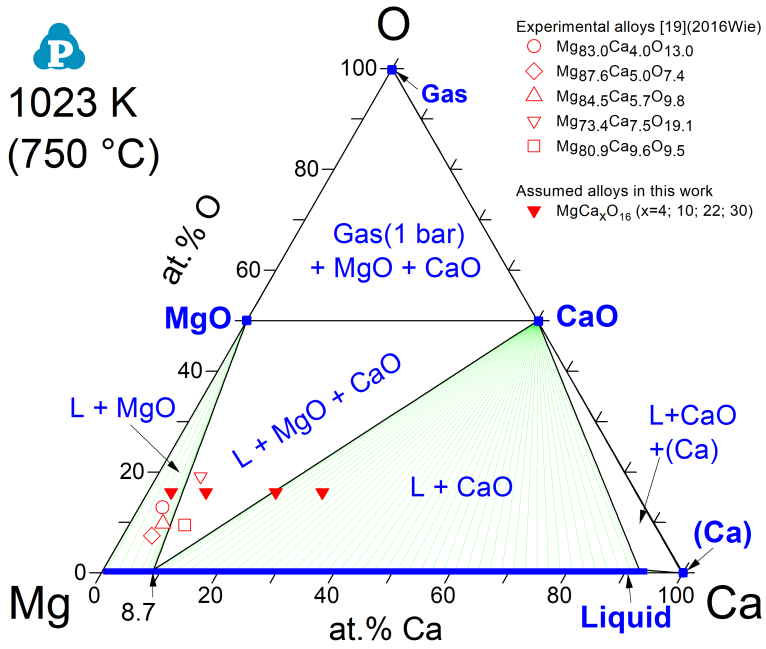


Figure 1.13: Calculated isothermal section of the Mg-Ca-O system, validated using in-situ synchrotron radiation diffraction [2018Lia1]

The good agreement between experimental and calculated results, as shown in all of the above figures indicates the reliability of the current PanMagnesium thermodynamic database. Additional validation is given in some comprehensive studies [2012Sch, 2013Gro]. Applications are highlighted in [2018Sch].

2 Mobility Database

PanMg2025_MB is an atomic mobility database for Mg-based alloys, which is compatible with the `PanMg2025_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

	Ag	Al	Bi	Ca	Ce	Co	Cu	Dy	Er	Fe	Gd	La	Li	Mg	Mn	Nd	Ni	Pr
Bcc																		
Fcc																		
Hcp																		

	Sc	Se	Si	Sn	Sr	Y	Zn	Zr
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 `PanMg2025_MB` database are also assessed. In the following, the assessed chemical-diffusivity within the binary and ternary systems for the Fcc, and Hcp phases are listed, respectively.

Fcc Phase

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

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

Hcp phase

Al-Mg	Mg-Zn	Al-Mg-Zn

2.4 Database Validation

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

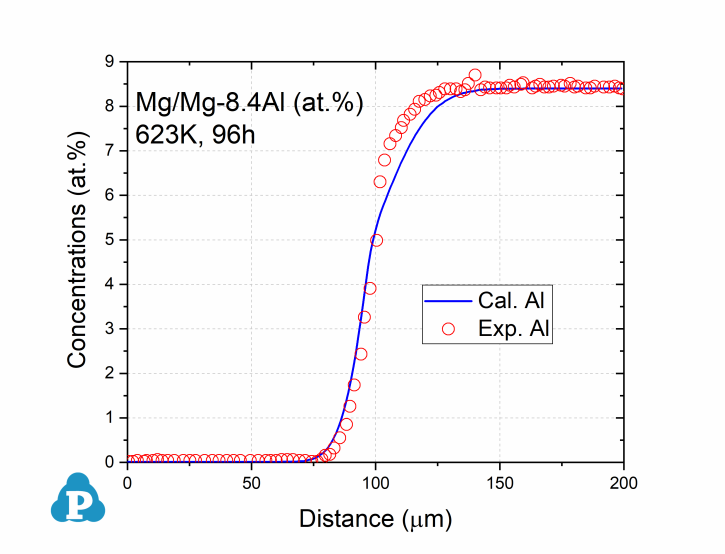


Figure 2.1: Concentration profile of Mg/Mg-8.4Al (at.%) annealed at 623K for 96h with data [2014Kam]

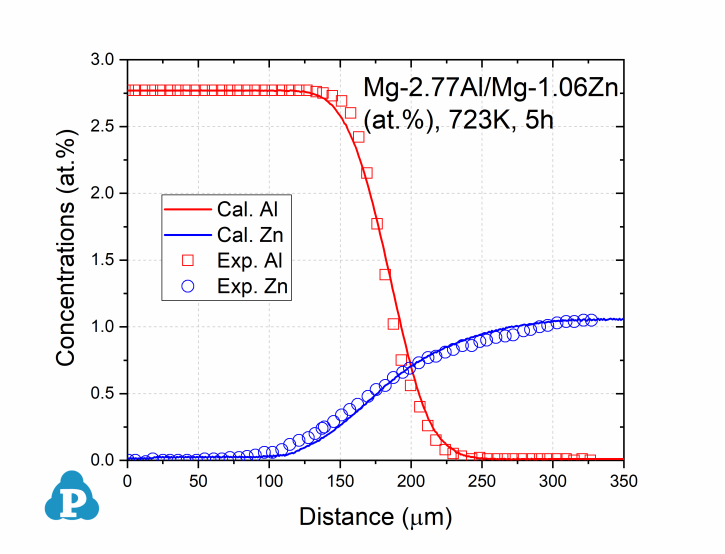


Figure 2.2: Concentration profile of Mg-2.77Al/Mg-1.06Zn (at.%) annealed at 723K for 5h [2016Kam]

2.5 Applications

This mobility database is combined with the thermodynamic database for Al-based alloys, `PanMg_TH`, to simulate the diffusion-controlled phenomena of Mg-based alloys. A few examples are given below.

2.5.1 Precipitation kinetics of magnesium alloys

The **PanEvolution** module was developed for the simulation of precipitation kinetics of multi-component alloys. It has been seamlessly integrated with the thermodynamic calculation engine of Pandat software, and has been used to simulate the evolution of microstructure and the corresponding mechanical property responses to heat treatment magnesium alloys [2011Cao]. Below shows an example simulation performed for the AZ91 alloy. Figure 2.3 shows the simulated particle size evolution with time of the γ-Mg17Al12 precipitate aged at 200 °C compared with the experimental data of [2001Cel]. Figure 2.4 shows yield strength evolution with time. As is seen, the particles grow and coarsen with ageing time, while the yield strength reaches peak at a time varies with heat treatment temperature. The database used to do this simulation is the combined thermodynamic and mobility database of Mg-based alloys: `PanMg_TH+MB`. More information regarding to precipitation simulation can be found in PanEvolution module under the Software section.

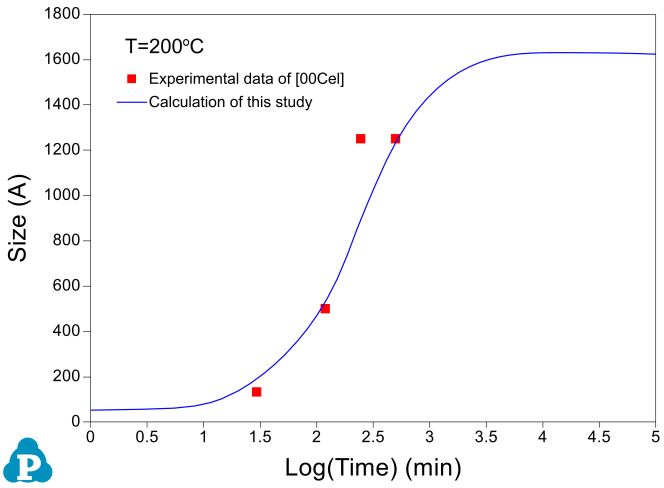


Figure 2.3: Calculated particle size evolution of the γ-$Mg_{17}Al_{12}$ precipitate aged at 200 °C compared with the experimental data of [2001Cel]

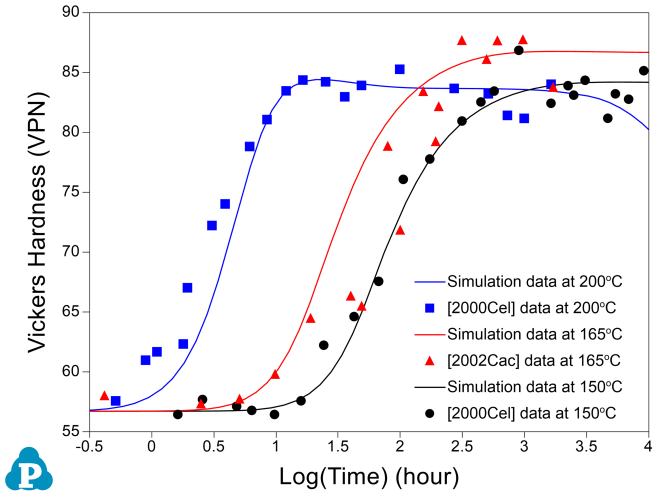


Figure 2.4: Simulated hardness curves of AZ91 alloy aged at 150, 165 and 200 °C compared with the experimentally measured data of [2001Cel, 2002Cac]

2.5.2 Solidification of magnesium alloys

The combined thermodynamic and mobility database of Mg-based alloys: `PanMg_TH+MB` is also used to simulate the solidification process considering back diffusion in the solid phase [2019Zha]. Figure 2.5 compares the simulated and measured [2013Pal] Al composition profiles in the α(Mg) phase vs. fraction of solid (fs) for Mg-*x*Al (*x*=3, 6 ,9) alloys. Figure 2.6 compares the simulated and measured secondary dendrite arm spacing (SDAS) [2013Pal2] results of Mg-Al binary alloys. More information regarding to solidification simulation can be found in PanSolidification module under the Software section.

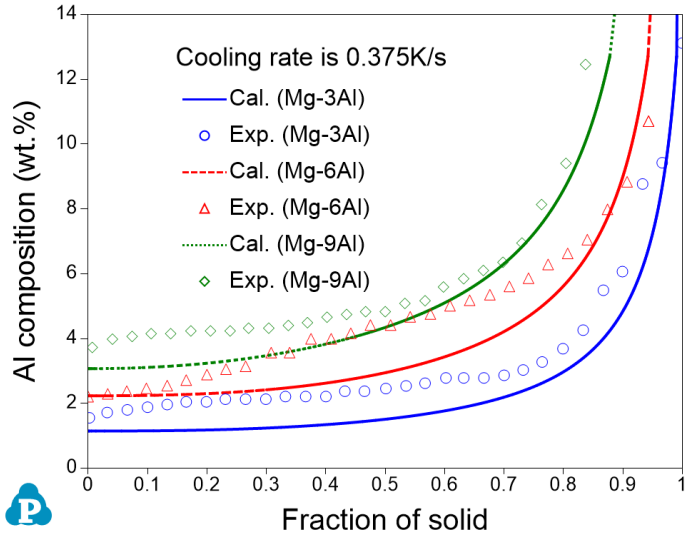


Figure 2.5: Comparison between the simulated and measured [2013Pal] Al composition profiles in the hcp_α(Mg) phase vs. fs for Mg-*x*Al (*x*=3, 6 ,9) alloys

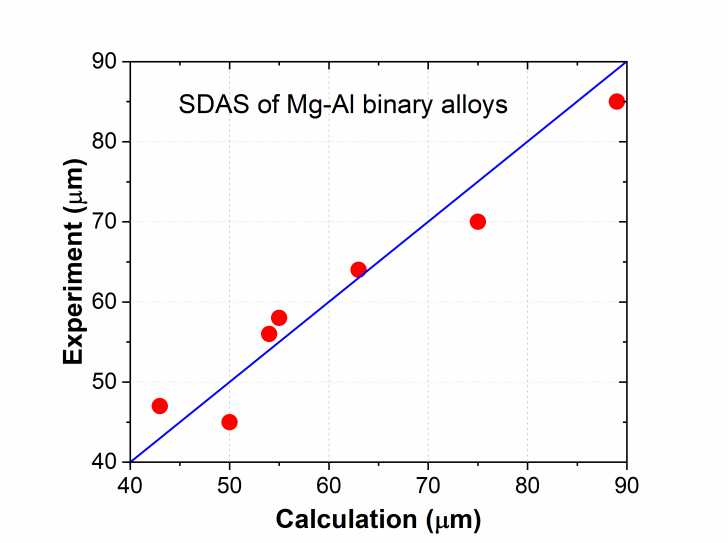


Figure 2.6: Comparison between the simulated and measured SDAS [2013Pal2] for Mg-Al binary alloys

3 Thermophysical Property Database

The thermophysical property database **PanMg2025_ TP** is compatible with the `PanMg2025_TH` thermodynamic database and suitable for the simulation of thermophysical properties of Mg-based alloys. It includes the molar volume data for all the phases, surface tension and viscosity properties for the liquid phase, and thermal conductivity database, which can be used to calculate the thermal conductivity of the alloys under equilibrium, as-cast and as quenched three types of conditions.

3.1 Molar Volume

The current molar volume database covers all **854** phases assessed in the `PanMg2025_TH` database. It is used to calculate the density, thermal expansion, solidification shrinkage of Fe-based alloys.

The simulated density changes vs. temperature of a series of Mg-based alloys are shown below to validate the current `PanMg2025_MV` database.

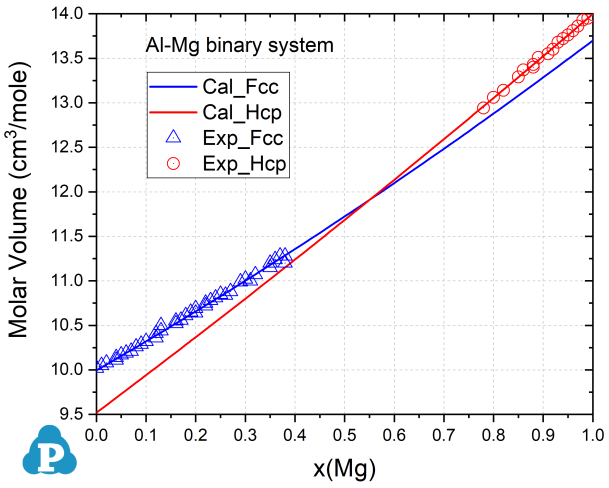


Figure 3.1: Molar volume of Al-Mg Fcc and Hcp binary alloys at 298K [2000Gas, 2006Hal]

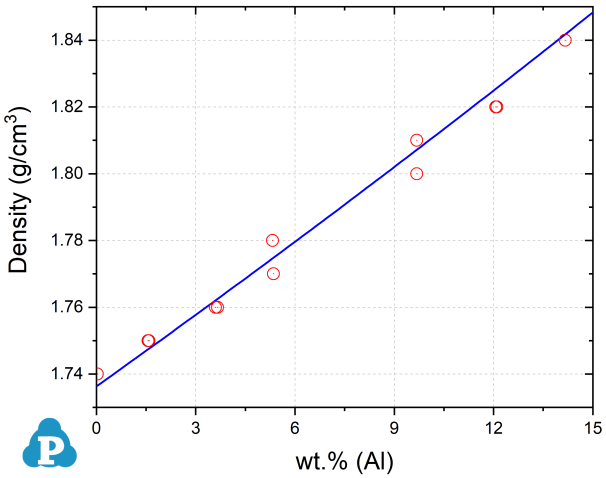


Figure 3.2: Density of Mg-Al binary alloys at 298K [2000Gas, 2006Hal]

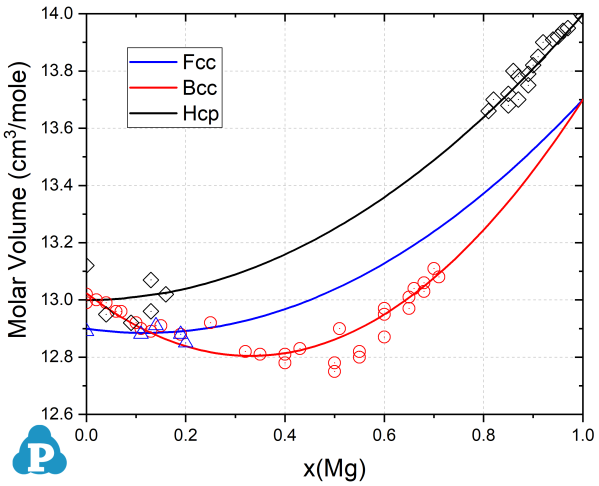


Figure 3.3: Molar volume of Li-Mg Bcc, Fcc, and Hcp binary alloys at 298K [1998Gas, 2006Hal]

3.2 Surface Tension

The surface tension of the liquid phase is added into the property database. Figure 3.4 shows the surface tension of a series of Mg-Al-Zn alloys in comparison with experimental data.

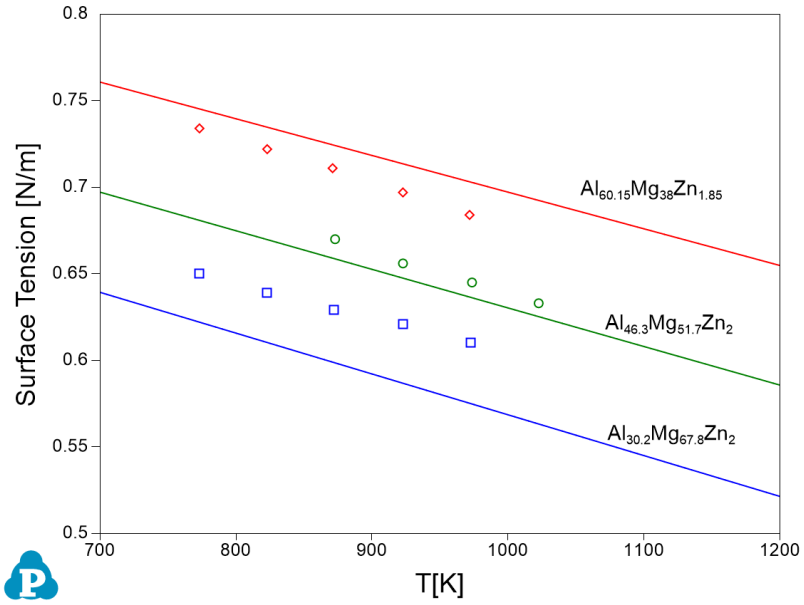


Figure 3.4: Surface tension of Mg-Al-Zn alloys

3.3 Viscosity

The viscosity of the liquid phase is added into the property database. Figure 3.5 shows the viscosity of a Mg30.2Al-25Zn alloy in comparison with experimental data.

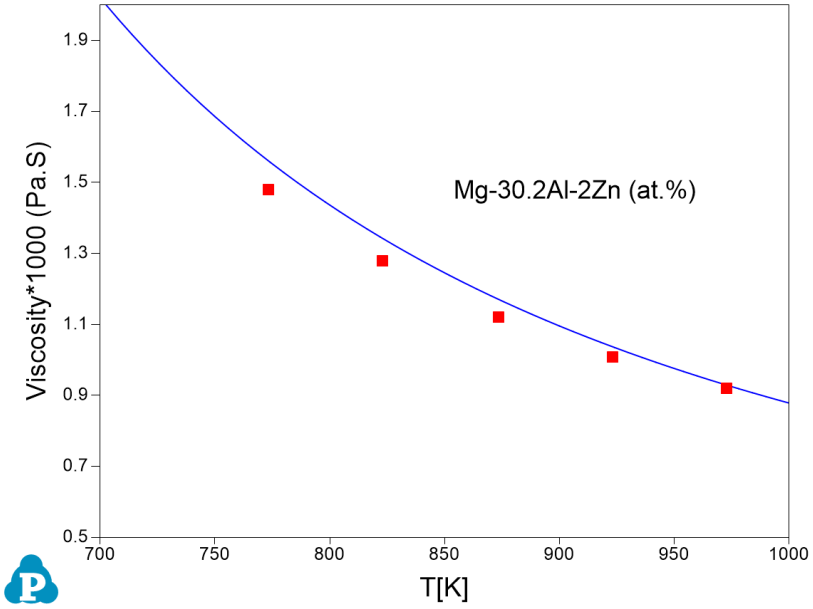


Figure 3.5: Viscosity of the Mg30.2Al-25Zn alloy

3.4 Thermal Conductivity

The calculated thermal conductivities of Mg Alloys under as-cast condition are in agreement with the measured values [2024Lv] as shown in Figure 3.6. The major discrepancy occurs when strong crystallographic texture results in anisotropy property in different directions like Mg-Mn-Zn related and some RE-related systems.

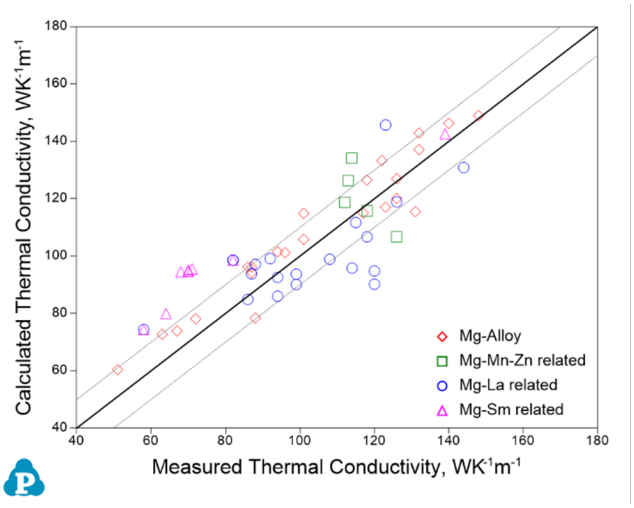


Figure 3.6: Comparison of calculated and measured thermal conductivity of Mg alloys in the as-cast condition

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PanMg2025:List of All Phases

Phases (**854**)

Name	Model	Lattice Size	Constituent
Ag2Ca	CEF (ST2)	(0.666667) (0.333333)	(Ag)(Ca)
Ag2Er	CEF (ST2)	(0.667) (0.333)	(Ag)(Er)
Ag2La	CEF (ST2)	(2)(1)	(Ag)(La)
Ag2O	CEF (ST2)	(2)(1)	(Ag)(O)
Ag2O2	CEF (ST2)	(2)(2)	(Ag)(O)
Ag2O3	CEF (ST2)	(2)(3)	(Ag)(O)
Ag2Sc	CEF (ST2)	(0.667) (0.333)	(Ag)(Sc)
Ag2Sm_T1	CEF (ST2)	(2)(1)	(Ag)(Sm)
Ag2Sm_T2	CEF (ST2)	(2)(1)	(Ag)(Sm)
Ag2Sr	CEF (ST2)	(2)(1)	(Ag)(Sr)
Ag2Sr3	CEF (ST2)	(2)(3)	(Ag)(Sr)
Ag2Y	CEF (ST2)	(0.667) (0.333)	(Ag)(Y)
Ag3Ca5	CEF (ST2)	(0.375) (0.625)	(Ag)(Ca)

Name	Model	Lattice Size	Constituent
Ag3Sb	CEF (SLN)	(0.75)(0.25)	(Ag,Sb)(Ag,Sb)
Ag3Sn	CEF (SLN)	(0.75)(0.25)	(Ag)(Ag,Sn)
Ag4Sc	CEF (ST2)	(0.8)(0.2)	(Ag)(Sc)
Ag4Sr	CEF (ST2)	(4)(1)	(Ag)(Sr)
Ag51Er14	CEF (SLN)	(0.785) (0.215)	(Ag,Er)(Er)
Ag51La14	CEF (ST2)	(51)(14)	(Ag)(La)
Ag51Sm14	CEF (ST2)	(0.784615) (0.21385)	(Ag)(Sm)
Ag51Y14	CEF (ST2)	(0.785) (0.215)	(Ag)(Y)
Ag5La	CEF (ST2)	(5)(1)	(Ag)(La)
Ag5Sr	CEF (ST2)	(5)(1)	(Ag)(Sr)
Ag5Zn8	CEF (SLN)	(2)(2)(3)(6)	(Ag,Zn)(Ag)(Ag,Zn)(Ag,Zn)
Ag7Ca2	CEF (ST2)	(0.777778) (0.222222)	(Ag)(Ca)
Ag9Ca2	CEF (ST2)	(0.818182) (0.181818)	(Ag)(Ca)
AgAl6Mg4	CEF (SLN)	(0.605) (0.395)	(Ag,Al)(Mg)
AgAlMg	CEF (ST3)	(0.33333) (0.33333) (0.33333)	(Ag)(Al)(Mg)

Name	Model	Lattice Size	Constituent
AgCa	CEF (ST2)	(0.5)(0.5)	(Ag)(Ca)
AgCa3	CEF (ST2)	(0.25)(0.75)	(Ag)(Ca)
AgEr	CEF (ST2)	(1)(1)	(Ag)(Er)
AgLaMg	CEF (ST3)	(1)(1)(1)	(Ag)(La)(Mg)
AgMg3	CEF (SLN)	(0.23)(0.77)	(Ag,Cu)(Al,Mg)
AgMg4	CEF (SLN)	(0.2)(0.8)	(Ag,Cu)(Al,Mg)
AgMgSb_T1	CEF (ST3)	(1)(1)(1)	(Ag)(Mg)(Sb)
AgMgSb_T2	CEF (ST3)	(1)(1)(1)	(Ag)(Mg)(Sb)
AgMgSb_T3	CEF (ST3)	(1)(1)(1)	(Ag)(Mg)(Sb)
AgMg_L12	CEF (SLN)	(0.25)(0.25) (0.25)(0.25) (1)	(Ag,Al,Cu,Mg)(Ag,Al,Cu,Mg) (Ag,Al,Cu,Mg)(Ag,Al,Cu,Mg)(Va)
AgSc	CEF (ST2)	(0.5)(0.5)	(Ag)(Sc)
AgSm	CEF (ST2)	(0.5)(0.5)	(Ag)(Sm)
AgSr	CEF (ST2)	(1)(1)	(Ag)(Sr)
AgY	CEF (ST2)	(0.5)(0.5)	(Ag)(Y)
AgZn	CEF (SLN)	(1)(2)	(Zn)(Ag,Zn)
AgZn3	CEF (SLN)	(1)	(Ag,Zn)
AgZr	CEF (ST2)	(0.5)(0.5)	(Ag)(Zr)
AgZr2	CEF (ST2)	(0.333333) (0.666667)	(Ag)(Zr)

Name	Model	Lattice Size	Constituent
Al11Mn4_T1	CEF (SLN)	(11)(4)	(Al)(Fe,Mn)
Al11Mn4_T2	CEF (SLN)	(29)(10)	(Al,Mn)(Mn)
Al11Pr3	CEF (ST2)	(11)(3)	(Al)(Pr)
Al11Sm3	CEF (ST2)	(11)(3)	(Al)(Sm)
Al12Ca6Li11	CEF (ST3)	(0.206897) (0.37931) (0.413793)	(Ca)(Li)(Al)
Al12Mg17	CEF (SLN)	(10)(24)(24)	(Mg)(Al,Ca,Cu,Li,Mg,Zn) (Al,Cu,Mg,Zn)
Al12Mn	CEF (SLN)	(12)(1)	(Al)(Fe,Mn)
Al13Co4	CEF (SLN)	(0.6275) (0.235) (0.1375)	(Al)(Co)(Al,Va)
Al13Fe4	CEF (SLN)	(0.6275) (0.235) (0.1375)	(Al)(Fe,Mn)(Al,Si,Va)
Al14SiY5	CEF (ST3)	(14)(1)(5)	(Al)(Si)(Y)
Al17Cu9Mg45Si29	CEF (ST4)	(0.17)(0.09) (0.45)(0.29)	(Al)(Cu)(Mg)(Si)
Al18Mg3Mn2	CEF (ST3)	(18)(3)(2)	(Al)(Mg)(Mn)
Al18Mn4Si	CEF (SLN)	(16)(4)(1)(2)	(Al)(Mn)(Si)(Al,Si)
Al19Mn6Si	CEF (SLN)	(15)(1)(4)(6)	(Al)(Si)(Al,Si)(Mn)

Name	Model	Lattice Size	Constituent
Al20Sm4_thta	CEF (ST2)	(20)(4)	(Al)(Sm)
Al23Cu77	CEF (ST2)	(0.23)(0.77)	(Al)(Cu)
Al29Cu4Mn6	CEF (ST3)	(29)(4)(6)	(Al)(Cu)(Mn)
Al2CaSi2	CEF (ST3)	(0.4)(0.2)(0.4)	(Al)(Ca)(Si)
Al2Ca_C15	CEF (SLN)	(0.666667) (0.333333)	(Al,Mg)(Ca,Sr)
Al2Cu	CEF (SLN)	(2)(1)	(Al)(Al,Cu)
Al2CuLi	CEF (ST3)	(0.5)(0.25) (0.25)	(Al)(Cu)(Li)
Al2CuMg	CEF (ST3)	(2)(1)(1)	(Al)(Cu)(Mg)
Al2Er3	CEF (ST2)	(0.4)(0.6)	(Al)(Er)
Al2Er_C15	CEF (SLN)	(2)(1)	(Al,Er)(Al,Er)
Al2Fe	CEF (SLN)	(2)(1)	(Al)(Fe,Mn)
Al2Li3	CEF (ST2)	(2)(3)	(Al)(Li)
Al2MgC2	CEF (ST3)	(2)(1)(2)	(Al)(Mg)(C)
Al2MgO4	CEF (ST3)	(2)(1)(4)	(Al)(Mg)(O)
Al2MnSi3	CEF (ST3)	(2)(1)(3)	(Al)(Mn)(Si)
Al2O3	CEF (ST2)	(2)(3)	(Al)(O)
Al2Pr	CEF (ST2)	(2)(1)	(Al)(Pr)
Al2Sc_C15	CEF (SLN)	(0.666667) (0.333333)	(Al,Mg)(Sc)

Name	Model	Lattice Size	Constituent
Al2Si2Sr	CEF (ST3)	(2)(2)(1)	(Al)(Si)(Sr)
Al2Si2Y	CEF (ST3)	(2)(2)(1)	(Al)(Si)(Y)
Al2Sm	CEF (ST2)	(2)(1)	(Al)(Sm)
Al2Sr	CEF (SLN)	(2)(1)	(Al,Mg)(Ca,Sr)
Al2Y3	CEF (SLN)	(2)(3)	(Al,Mg)(Y)
Al2Zr3	CEF (ST2)	(0.4)(0.6)	(Al)(Zr)
Al2Zr_C14	CEF (ST2)	(0.666667) (0.333333)	(Al)(Zr)
Al30Mg23	CEF (SLN)	(23)(30)	(Mg)(Al,Cu,Zn)
Al35Fe37Si28	CEF (ST3)	(0.35)(0.37) (0.28)	(Al)(Fe)(Si)
Al38Mg58Sr4	CEF (ST3)	(38)(58)(4)	(Al)(Mg)(Sr)
Al3Ca8	CEF (SLN)	(0.272727) (0.727272)	(Al)(Ca,Mg)
Al3Co	CEF (ST2)	(3)(1)	(Al)(Co)
Al3Er	CEF (ST2)	(0.75)(0.25)	(Al)(Er)
Al3Li8Si5	CEF (ST3)	(8)(3)(5)	(Li)(Al)(Si)
Al3Mg2	CEF (SLN)	(89)(140)	(Mg,Li)(Al,Cu,Zn)
Al3Ni	CEF (ST2)	(0.75)(0.25)	(Al)(Ni)
Al3Ni2	CEF (SLN)	(3)(2)(1)	(Al)(Al,Ni)(Ni,Va)
Al3Ni5	CEF (ST2)	(0.375)	(Al)(Ni)

Name	Model	Lattice Size	Constituent
		(0.625)	
Al3Ni_L12	CEF (SLN)	(0.75)(0.25) (1)	(Al,Ni)(Al,Ni)(Va)
Al3Pr	CEF (ST2)	(3)(1)	(Al)(Pr)
Al3Sc	CEF (SLN)	(0.75)(0.25)	(Al,Mg)(Sc)
Al3Sm	CEF (ST2)	(3)(1)	(Al)(Sm)
Al3Sr8	CEF (ST2)	(3)(8)	(Al)(Sr)
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)
Al40Fe25Si35	CEF (ST3)	(0.4)(0.25) (0.35)	(Al)(Fe)(Si)
Al41Sm5_eta	CEF (ST2)	(41)(5)	(Al)(Sm)
Al461Mn107	CEF (ST2)	(461)(107)	(Al)(Mn)
Al49Fe16Si35	CEF (ST3)	(0.49)(0.16) (0.35)	(Al)(Fe)(Si)
Al4C3	CEF (SLN)	(2)(2)(3)	(Al,Mg)(Al)(C)
Al4Ca	CEF (SLN)	(0.8)(0.2)	(Al,Mg)(Ca,Sr)

Name	Model	Lattice Size	Constituent
Al4Li9	CEF (ST2)	(4)(9)	(Al)(Li)
Al4MgY_C14	CEF (ST3)	(4)(1)(1)	(Al)(Mg)(Y)
Al4Mn	CEF (SLN)	(4)(1)	(Al)(Fe,Mn)
Al4SiC4	CEF (ST3)	(4)(1)(4)	(Al)(Si)(C)
Al4Sr	CEF (SLN)	(4)(1)	(Al,Mg)(Ca,Sr)
Al4Zr5	CEF (ST2)	(0.444444) (0.555556)	(Al)(Zr)
Al53Li33Mg14	CEF (ST3)	(0.53)(0.33) (0.14)	(Al)(Li)(Mg)
Al54Fe26Si20	CEF (ST3)	(0.54)(0.26) (0.2)	(Al)(Fe)(Si)
Al55Cu11Li33	CEF (ST3)	(0.55)(0.117) (0.333)	(Al)(Cu)(Li)
Al57Cu11Li32	CEF (ST3)	(0.57)(0.11) (0.32)	(Al)(Cu)(Li)
Al5Co2	CEF (ST2)	(5)(2)	(Al)(Co)
Al5Cu4Zn	CEF (SLN)	(1)(4)(4)(1)	(Al,Cu)(Al)(Cu)(Zn)
Al5Cu8	CEF (ST2)	(5)(8)	(Al)(Cu)
Al5Fe2	CEF (SLN)	(5)(2)	(Al)(Fe,Mn)
Al5Fe4	CEF (SLN)	(1)	(Al,Fe)
Al60Cu32Li8	CEF (ST3)	(0.6)(0.32) (0.08)	(Al)(Cu)(Li)

Name	Model	Lattice Size	Constituent
Al60Fe15Si25	CEF (SLN)	(0.598) (0.152)(0.1) (0.15)	(Al)(Fe)(Si)(Al,Si)
Al60Sm11_eps	CEF (ST2)	(60)(11)	(Al)(Sm)
Al64Fe20Si16	CEF (ST3)	(0.635) (0.205)(0.16)	(Al)(Fe)(Si)
Al66Fe19Si15	CEF (SLN)	(0.66)(0.19) (0.05)(0.1)	(Al)(Fe)(Si)(Al,Si)
Al6Mn	CEF (SLN)	(6)(1)	(Al)(Fe,Mn)
Al7Cu3Mg6	CEF (ST3)	(7)(3)(6)	(Al)(Cu)(Mg)
Al7Sr8	CEF (SLN)	(7)(8)	(Al)(Ca,Sr)
Al8FeMg3Si6	CEF (ST4)	(8)(3)(1)(6)	(Al)(Mg)(Fe)(Si)
Al8Mn4RE	CEF (SLN)	(8)(4)(1)	(Al)(Mn)(Ce,Gd,Nd,Sm)
Al8Mn5	CEF (SLN)	(12)(5)(9)	(Al)(Mn)(Al,Fe,Mn)
Al8SiC7	CEF (ST3)	(8)(1)(7)	(Al)(Si)(C)
Al9Co2	CEF (ST2)	(9)(2)	(Al)(Co)
Al9Cu11	CEF (SLN)	(9)(11)	(Al,Cu)(Cu)
AlCa	CEF (ST2)	(0.5)(0.5)	(Al)(Ca)
AlCaLi_C36	CEF (SLN)	(0.333333) (0.666667)	(Ca)(Li,Al)
AlCaMg_C36	CEF (SLN)	(0.48) (0.186667)	(Al)(Al,Mg)(Ca,Mg)

Name	Model	Lattice Size	Constituent
		(0.333333)	
AlCu3Mn2_C15	CEF (ST3)	(0.5)(0.333) (0.167)	(Cu)(Mn)(Al)
AlCu_eps	CEF (SLN)	(1)(1)	(Al,Cu,Zn)(Cu)
AlCu_eta	CEF (ST2)	(0.48)(0.52)	(Al)(Cu)
AlCu_eta1	CEF (SLN)	(1)(1)	(Al,Cu)(Cu,Zn)
AlCu_gam1	CEF (SLN)	(4)(6)(16)	(Cu)(Cu,Zn)(Ag,Al,Cu,Mn,Zn)
AlEr	CEF (ST2)	(0.5)(0.5)	(Al)(Er)
AlEr2	CEF (ST2)	(0.333) (0.667)	(Al)(Er)
AlLi	CEF (SLN)	(1)(1)	(Al,Li,Mg)(Li,Mg,Va)
AlLi5Si2	CEF (ST3)	(5.3)(0.7)(2)	(Li)(Al)(Si)
AlLiSi	CEF (ST3)	(1)(1)(1)	(Li)(Al)(Si)
AlMgZn_phi	CEF (SLN)	(6)(5)	(Mg)(Al,Cu,Zn)
AlMgZn_tau	CEF (SLN)	(26)(6)(48)(1)	(Mg)(Al,Mg)(Al,Cu,Mg,Zn)(Al)
AlNi_B2	CEF (SLN)	(1)(1)	(Al,Co,Ni,Va)(Al,Co,Ni,Va)
AlP	CEF (ST2)	(1)(1)	(Al)(P)
AlPr	CEF (ST2)	(1)(1)	(Al)(Pr)
AlPr2	CEF (ST2)	(1)(2)	(Al)(Pr)
AlPr3	CEF (ST2)	(1)(3)	(Al)(Pr)

Name	Model	Lattice Size	Constituent
AlSb	CEF (ST2)	(0.5)(0.5)	(Al)(Sb)
AlSc	CEF (SLN)	(0.5)(0.5)	(Al,Mg)(Sc)
AlSc2	CEF (ST2)	(0.333333) (0.666667)	(Al)(Sc)
AlSm	CEF (ST2)	(1)(1)	(Al)(Sm)
AlSm2	CEF (ST2)	(1)(2)	(Al)(Sm)
AlY	CEF (ST2)	(1)(1)	(Al)(Y)
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)
Bcc	CEF (SLN)	(1)(3)	(Ag,Al,Ca,Ce,Co,Cu,Dy,Er,Fe, Gd,La,Li,Mg,Mn,Nd,Ni,Pr,Sb, Sc,Si,Sm,Sn,Sr,Y,Zn,Zr)(Va)
Bcc_B2	CEF (SLN)	(0.5)(0.5)(3)	(Ag,Al,Cu,Er,Fe,Mg,Mn,Si, Sm,Zn) (Ag,Al,Cu,Er,Fe,Mg,Mn, Si,Sm,Zn)(Va)
Bct	CEF (SLN)	(1)	(Ag,Al,Bi,Sb,Sn,Zn)
Bi2Mg3_T1	CEF (SLN)	(2)(3)	(Bi,Sn,Va)(Mg)
Bi2Mg3_T2	CEF (SLN)	(1)(3)(6)	(Bi,Sn)(Bi,Sn,Va)(Mg)
Bi2O3	CEF (ST2)	(2)(3)	(Bi)(O)
C_graph	CEF (ST1)	(1)	(C)

Name	Model	Lattice Size	Constituent
Ca11Sb10	CEF (ST2)	(11)(10)	(Ca)(Sb)
Ca14Si19	CEF (ST2)	(0.424242) (0.575757)	(Ca)(Si)
Ca156Mg94Sn175	CEF (ST3)	(156)(94) (175)	(Ca)(Mg)(Sn)
Ca22Li25Si53	CEF (ST3)	(1.65)(1.85) (4)	(Ca)(Li)(Si)
Ca2Cu	CEF (ST2)	(0.666667) (0.333333)	(Ca)(Cu)
Ca2Li5Si3	CEF (ST3)	(2)(5)(3)	(Ca)(Li)(Si)
Ca2LiSi	CEF (ST3)	(2)(1)(1)	(Ca)(Li)(Si)
Ca2LiSi3	CEF (ST3)	(2)(1)(3)	(Ca)(Li)(Si)
Ca2Mg55Zn43_im4	CEF (ST3)	(2)(55)(43)	(Ca)(Mg)(Zn)
Ca2Mg5Zn13_im3	CEF (ST3)	(2)(5)(13)	(Ca)(Mg)(Zn)
Ca2Mg5Zn5_im1	CEF (SLN)	(1)(1)(1)(3)	(Ca)(Mg)(Zn)(Mg,Zn)
Ca2Mg6Zn3_im0	CEF (ST3)	(2)(6)(3)	(Ca)(Mg)(Zn)
Ca2Ni7	CEF (ST2)	(0.222222) (0.777778)	(Ca)(Ni)
Ca2Sb	CEF (ST2)	(2)(1)	(Ca)(Sb)
Ca2Si	CEF (ST2)	(0.666667) (0.333333)	(Ca)(Si)
Ca2Sn	CEF (SLN)	(1)(1)(1)	(Ca,Mg)(Ca,Ce)(Sn,Si)

Name	Model	Lattice Size	Constituent
Ca31Sn20	CEF (ST2)	(31)(20)	(Ca)(Sn)
Ca36Sn23	CEF (ST2)	(36)(23)	(Ca)(Sn)
Ca3P2	CEF (ST2)	(3)(2)	(Ca)(P)
Ca3Si4	CEF (ST2)	(0.428571) (0.571428)	(Ca)(Si)
Ca3Zn	CEF (ST2)	(3)(1)	(Ca)(Zn)
Ca5Sb3	CEF (ST2)	(5)(3)	(Ca)(Sb)
Ca5Si3	CEF (ST2)	(0.625) (0.375)	(Ca)(Si)
Ca5Sn3	CEF (ST2)	(5)(3)	(Ca)(Sn)
Ca5Zn3	CEF (ST2)	(5)(3)	(Ca)(Zn)
Ca7Mg6Si14	CEF (ST3)	(7)(6)(14)	(Ca)(Mg)(Si)
Ca7Mg8Zn35_im2	CEF (ST3)	(7)(8)(35)	(Ca)(Mg)(Zn)
Ca7Sn6	CEF (ST2)	(7)(6)	(Ca)(Sn)
CaC2_T1	CEF (ST2)	(2)(1)	(C)(Ca)
CaC2_T2	CEF (ST2)	(2)(1)	(C)(Ca)
CaCu	CEF (ST2)	(0.5)(0.5)	(Ca)(Cu)
CaCu5	CEF (SLN)	(0.166667) (0.833333)	(Ca,Ce,La,Gd,Nd,Y)(Al,Cu,Ni)
CaLi2Si	CEF (ST3)	(1)(2)(1)	(Ca)(Li)(Si)
CaLiSi2	CEF (ST3)	(1)(1)(2)	(Ca)(Li)(Si)

Name	Model	Lattice Size	Constituent
CaMg2_C14	CEF (SLN)	(0.333333) (0.666667)	(Ca,Sr)(Li,Mg,Al,Zn)
CaMgSi	CEF (SLN)	(1)(1)(1)	(Ca)(Ca,Mg)(Si,Sn)
CaNi2_C15	CEF (ST2)	(0.333333) (0.666667)	(Ca)(Ni)
CaNi3	CEF (ST2)	(0.25)(0.75)	(Ca)(Ni)
CaO2	CEF (ST2)	(1)(2)	(Ca)(O)
CaSb2	CEF (ST2)	(1)(2)	(Ca)(Sb)
CaSi	CEF (ST2)	(0.5)(0.5)	(Ca)(Si)
CaSi2	CEF (ST2)	(0.333333) (0.666667)	(Ca)(Si)
CaSn	CEF (ST2)	(1)(1)	(Ca)(Sn)
CaSn3	CEF (ST2)	(1)(3)	(Ca)(Sn)
CaZn	CEF (ST2)	(1)(1)	(Ca)(Zn)
CaZn11	CEF (ST2)	(1)(11)	(Ca)(Zn)
CaZn13	CEF (SLN)	(1)(13)	(Ca,Sr)(Zn)
CaZn2	CEF (SLN)	(1)(2)	(Ca,Sr)(Zn)
CaZn3	CEF (ST2)	(1)(3)	(Ca)(Zn)
CaZn5	CEF (SLN)	(1)(5)	(Ca,Sr)(Zn)
Cbcc	CEF (SLN)	(1)(1)	(Al,Ce,Co,Cu,Fe,Mg,Mn, Ni,Si,Sn,Zn)(Va)

Name	Model	Lattice Size	Constituent
Ce10Al16Si4	CEF (ST3)	(0.533333) (0.333333) (0.133333)	(Al)(Ce)(Si)
Ce11Sn10	CEF (SLN)	(0.429) (0.429) (0.142)	(Ce)(Sn)(Ce,Sn)
Ce14Ag51	CEF (ST2)	(0.784615) (0.215385)	(Ag)(Ce)
Ce18O31	CEF (ST2)	(18)(31)	(Ce)(O)
Ce2Fe17	CEF (ST2)	(2)(17)	(Ce)(Fe)
Ce2Mg53Zn45_t2	CEF (ST3)	(0.02)(0.53) (0.45)	(Ce)(Mg)(Zn)
Ce2O3	CEF (ST2)	(2)(3)	(Ce)(O)
Ce2Sb	CEF (ST2)	(2)(1)	(Ce)(Sb)
Ce2Sn5	CEF (ST2)	(0.286) (0.714)	(Ce)(Sn)
Ce3Sn	CEF (ST2)	(0.75)(0.25)	(Ce)(Sn)
Ce3Sn5	CEF (ST2)	(0.375) (0.625)	(Ce)(Sn)
Ce3Sn7	CEF (ST2)	(0.3)(0.7)	(Ce)(Sn)
Ce4Sb3	CEF (ST2)	(4)(3)	(Ce)(Sb)
Ce5Sn3	CEF (ST2)	(0.625) (0.375)	(Ce)(Sn)

Name	Model	Lattice Size	Constituent
Ce5Sn4	CEF (ST2)	(0.556) (0.444)	(Ce)(Sn)
Ce6O11	CEF (ST2)	(6)(11)	(Ce)(O)
CeAg	CEF (ST2)	(0.5)(0.5)	(Ag)(Ce)
CeAg2	CEF (ST2)	(0.666667) (0.333333)	(Ag)(Ce)
CeAg4	CEF (ST2)	(0.8)(0.2)	(Ag)(Ce)
CeAl13Mg6_C14	CEF (ST3)	(13)(1)(6)	(Al)(Ce)(Mg)
CeAlSi2	CEF (ST3)	(0.25)(0.25) (0.5)	(Al)(Ce)(Si)
CeFe2	CEF (ST2)	(1)(2)	(Ce)(Fe)
CeMg12Zn_t1	CEF (SLN)	(1)(12)	(Ce)(Mg,Zn)
CeMg3Zn_t3	CEF (SLN)	(1)(3)	(Ce)(Mg,Zn)
CeMgZn_t4	CEF (ST3)	(0.125) (0.3125) (0.5625)	(Ce)(Mg)(Zn)
CeMgZn_t5	CEF (ST3)	(0.065) (0.283) (0.652)	(Ce)(Mg)(Zn)
CeO2	CEF (ST2)	(1)(2)	(Ce)(O)
CeSb	CEF (ST2)	(1)(1)	(Ce)(Sb)
CeSb2	CEF (ST2)	(1)(2)	(Ce)(Sb)

Name	Model	Lattice Size	Constituent
CeSn3	CEF (ST2)	(0.25)(0.75)	(Ce)(Sn)
Co11Ce24	CEF (ST2)	(11)(24)	(Co)(Ce)
Co11Zr2	CEF (ST2)	(11)(2)	(Co)(Zr)
Co12Zn88	CEF (ST2)	(0.117647) (0.882353)	(Co)(Zn)
Co13La	CEF (ST2)	(0.929) (0.071)	(Co)(La)
Co17Ce2	CEF (ST2)	(17)(2)	(Co)(Ce)
Co17Er2	CEF (ST2)	(17)(2)	(Co)(Er)
Co17Nd2	CEF (ST2)	(17)(2)	(Co)(Nd)
Co17Pr2	CEF (SLN)	(0.895) (0.105)	(Co,Pr)(Co,Pr)
Co17Sm2	CEF (SLN)	(0.833333) (0.111111) (0.055556)	(Co)(Sm)(Co2,Sm)
Co17Y2	CEF (ST2)	(17)(2)	(Co)(Y)
Co19Ce5	CEF (ST2)	(19)(5)	(Co)(Ce)
Co19La5	CEF (ST2)	(0.792) (0.208)	(Co)(La)
Co19Nd5	CEF (ST2)	(19)(5)	(Co)(Nd)
Co19Pr5	CEF (SLN)	(0.792) (0.208)	(Co,Pr)(Co,Pr)

Name	Model	Lattice Size	Constituent
Co19Sm5	CEF (ST2)	(0.791667) (0.208333)	(Co)(Sm)
Co23La27	CEF (ST2)	(0.46)(0.54)	(Co)(La)
Co23Zr6	CEF (ST2)	(23)(6)	(Co)(Zr)
Co2Ce	CEF (ST2)	(2)(1)	(Co)(Ce)
Co2Er	CEF (ST2)	(2)(1)	(Co)(Er)
Co2Gd	CEF (ST2)	(2)(1)	(Co)(Gd)
Co2Nd	CEF (ST2)	(2)(1)	(Co)(Nd)
Co2Nd5	CEF (ST2)	(2)(5)	(Co)(Nd)
Co2Pr	CEF (SLN)	(0.667) (0.333)	(Co,Pr)(Co,Pr)
Co2Pr5	CEF (ST2)	(0.286) (0.714)	(Co)(Pr)
Co2Sc	CEF (SLN)	(0.67)(0.33)	(Co,Sc)(Co,Sc)
Co2Si_T1	CEF (SLN)	(2)(1)	(Co,Si)(Co,Si)
Co2Si_T2	CEF (SLN)	(2)(1)	(Co,Si)(Co,Si)
Co2Sm	CEF (ST2)	(0.666667) (0.333333)	(Co)(Sm)
Co2Sm5	CEF (ST2)	(0.285714) (0.714286)	(Co)(Sm)
Co2Y	CEF (ST2)	(2)(1)	(Co)(Y)

Name	Model	Lattice Size	Constituent
Co2Zr_C15	CEF (SLN)	(2)(1)	(Co,Zr)(Co,Zr)
Co3Ce	CEF (ST2)	(3)(1)	(Co)(Ce)
Co3Er	CEF (ST2)	(3)(1)	(Co)(Er)
Co3Gd	CEF (ST2)	(3)(1)	(Co)(Gd)
Co3Gd4	CEF (ST2)	(3)(4)	(Co)(Gd)
Co3La2	CEF (ST2)	(0.6)(0.4)	(Co)(La)
Co3Nd	CEF (ST2)	(3)(1)	(Co)(Nd)
Co3Nd2_T1	CEF (ST2)	(3)(2)	(Co)(Nd)
Co3Nd2_T2	CEF (ST2)	(3)(2)	(Co)(Nd)
Co3Nd4	CEF (ST2)	(3)(4)	(Co)(Nd)
Co3Pr	CEF (SLN)	(0.75)(0.25)	(Co,Pr)(Co,Pr)
Co3Pr4	CEF (ST2)	(0.459) (0.541)	(Co)(Pr)
Co3Si	CEF (ST2)	(0.75)(0.25)	(Co)(Si)
Co3Sm	CEF (ST2)	(0.75)(0.25)	(Co)(Sm)
Co3Sn2	CEF (SLN)	(1)(1)(0.5) (0.5)	(Co)(Sn)(Co,Va)(Co,Va)
Co3Y	CEF (ST2)	(3)(1)	(Co)(Y)
Co3Y2	CEF (ST2)	(3)(2)	(Co)(Y)
Co3Y4	CEF (ST2)	(3)(4)	(Co)(Y)

Name	Model	Lattice Size	Constituent
Co4Zn	CEF (SLN)	(1)(1)	(Co,Zn)(Va)
Co5Ce	CEF (ST2)	(5)(1)	(Co)(Ce)
Co5Er	CEF (ST2)	(5)(1)	(Co)(Er)
Co5La	CEF (ST2)	(0.833) (0.167)	(Co)(La)
Co5Nd	CEF (ST2)	(5)(1)	(Co)(Nd)
Co5Pr	CEF (SLN)	(0.833) (0.167)	(Co,Pr)(Co,Pr)
Co5Sm	CEF (SLN)	(0.833333) (0.166667)	(Co,Va)(Co2,Sm)
Co5Y	CEF (ST2)	(5)(1)	(Co)(Y)
Co5Y8	CEF (ST2)	(5)(8)	(Co)(Y)
Co7Ce2	CEF (ST2)	(7)(2)	(Co)(Ce)
Co7Er12	CEF (ST2)	(7)(12)	(Co)(Er)
Co7Er2	CEF (ST2)	(7)(2)	(Co)(Er)
Co7Gd2	CEF (ST2)	(7)(2)	(Co)(Gd)
Co7La2	CEF (ST2)	(0.777) (0.223)	(Co)(La)
Co7Nd2	CEF (ST2)	(7)(2)	(Co)(Nd)
Co7Pr2	CEF (SLN)	(0.778) (0.222)	(Co,Pr)(Co,Pr)
Co7Sm2	CEF (ST2)	(0.777778)	(Co)(Sm)

Name	Model	Lattice Size	Constituent
		(0.222222)	
Co7Y2	CEF (SLN)	(7)(2)	(Co)(Ce,Y)
Co7Y6	CEF (ST2)	(7)(6)	(Co)(Y)
CoEr3	CEF (ST2)	(1)(3)	(Co)(Er)
CoGd3	CEF (ST2)	(1)(3)	(Co)(Gd)
CoGd_Delta	CEF (SLN)	(1)(2)(15)	(Co2,Gd)(Co2,Gd)(Co)
CoLa3	CEF (ST2)	(0.25)(0.75)	(Co)(La)
CoNd3	CEF (ST2)	(1)(3)	(Co)(Nd)
CoPr3	CEF (ST2)	(0.25)(0.75)	(Co)(Pr)
CoSb	CEF (SLN)	(0.3333) (0.3333) (0.3333)	(Sb)(Co,Va)(Co,Va)
CoSb2	CEF (ST2)	(0.3333) (0.6667)	(Co)(Sb)
CoSb3	CEF (ST2)	(0.25)(0.75)	(Co)(Sb)
CoSc	CEF (ST2)	(0.52)(0.48)	(Co)(Sc)
CoSc2	CEF (ST2)	(0.33)(0.67)	(Co)(Sc)
CoSc3	CEF (ST2)	(0.23)(0.77)	(Co)(Sc)
CoSi	CEF (SLN)	(0.5)(0.5)	(Co,Si)(Co,Si)
CoSi2	CEF (ST2)	(1)(2)	(Co)(Si)
CoSm3	CEF (ST2)	(0.25)(0.75)	(Co)(Sm)

Name	Model	Lattice Size	Constituent
CoSn	CEF (ST2)	(0.5)(0.5)	(Co)(Sn)
CoSn2	CEF (ST2)	(0.333) (0.667)	(Co)(Sn)
CoSn3	CEF (ST2)	(0.25)(0.75)	(Co)(Sn)
CoY	CEF (ST2)	(1)(1)	(Co)(Y)
CoY3	CEF (ST2)	(1)(3)	(Co)(Y)
CoZn14	CEF (ST2)	(0.0714286) (0.928571)	(Co)(Zn)
CoZn7	CEF (ST2)	(0.125) (0.875)	(Co)(Zn)
CoZn_HT	CEF (SLN)	(1)(1)	(Co,Zn)(Va)
CoZr2	CEF (ST2)	(1)(2)	(Co)(Zr)
CoZr3	CEF (ST2)	(1)(3)	(Co)(Zr)
CoZr_B2	CEF (ST2)	(1)(1)	(Co)(Zr)
Cu10Sb3	CEF (ST2)	(0.77)(0.23)	(Cu)(Sb)
Cu10Sn3	CEF (SLN)	(1)	(Cu,Sn)
Cu10Zr7	CEF (ST2)	(10)(7)	(Cu)(Zr)
Cu16Mg6Si7	CEF (ST3)	(16)(6)(7)	(Cu)(Mg)(Si)
Cu17Sb3	CEF (ST2)	(0.85)(0.15)	(Cu)(Sb)
Cu19Si6	CEF (ST2)	(19)(6)	(Cu)(Si)
Cu2Er	CEF (ST2)	(0.6667)	(Cu)(Er)

Name	Model	Lattice Size	Constituent
		(0.3333)	
Cu2MgY2_t3	CEF (ST3)	(2)(1)(2)	(Cu)(Mg)(Y)
Cu2Mg_C15	CEF (SLN)	(1)(2)	(Al,Cu,Li,Mg,Ni,Si,Zn) (Al,Cu,Li,Mg,Ni,Si,Zn)
Cu2O	CEF (ST2)	(2)(1)	(Cu)(O)
Cu2Sb	CEF (ST2)	(0.67)(0.33)	(Cu)(Sb)
Cu2Sm	CEF (ST2)	(0.666667) (0.333333)	(Cu)(Sm)
Cu2Y	CEF (ST2)	(2)(1)	(Cu)(Y)
Cu33Si7	CEF (ST2)	(33)(7)	(Cu)(Si)
Cu3Mg2Si	CEF (ST3)	(3)(2)(1)	(Cu)(Mg)(Si)
Cu3Sb	CEF (ST2)	(0.75)(0.25)	(Cu)(Sb)
Cu3Sn	CEF (SLN)	(3)(1)	(Cu,Sn)(Cu,Sn)
Cu3Zn_delta	CEF (SLN)	(1)	(Al,Cu,Zn)
Cu41Sn11	CEF (SLN)	(41)(11)	(Cu,Sn)(Cu,Sn)
Cu4MgY_t2	CEF (ST3)	(4)(1)(1)	(Cu)(Mg)(Y)
Cu4Sb	CEF (ST2)	(0.8)(0.2)	(Cu)(Sb)
Cu4Si	CEF (ST2)	(4)(1)	(Cu)(Si)
Cu4Sm	CEF (ST2)	(0.8)(0.2)	(Cu)(Sm)
Cu51Zr14	CEF (SLN)	(51)(14)	(Cu)(Y,Zr)

Name	Model	Lattice Size	Constituent
Cu56Si11	CEF (ST2)	(56)(11)	(Cu)(Si)
Cu5Er	CEF (ST2)	(0.8333) (0.1667)	(Cu)(Er)
Cu5Mg13Y5_t6	CEF (ST3)	(5)(13)(5)	(Cu)(Mg)(Y)
Cu5Mg16Y5_t8	CEF (ST3)	(5)(16)(5)	(Cu)(Mg)(Y)
Cu5Mg8Y5_t5	CEF (ST3)	(5)(8)(5)	(Cu)(Mg)(Y)
Cu5Sm	CEF (ST2)	(0.833333) (0.166667)	(Cu)(Sm)
Cu5Sr	CEF (ST2)	(0.833333) (0.166667)	(Cu)(Sr)
Cu5Zr	CEF (SLN)	(5)(1)	(Cu)(Y,Zr)
Cu6Sm	CEF (ST2)	(0.857143) (0.142857)	(Cu)(Sm)
Cu6Sn5_T1	CEF (SLN)	(1)(1)(1)	(Cu)(Cu,Sn)(Sn)
Cu6Sn5_T2	CEF (SLN)	(1)(1)(1)	(Cu)(Cu,Sn)(Sn)
Cu6Y	CEF (SLN)	(5)(1)	(Cu)(Cu2,Y,Zr)
Cu75Sn25_gam	CEF (SLN)	(1)	(Cu,Sn)
Cu7Er2	CEF (ST2)	(0.7778) (0.2222)	(Cu)(Er)
Cu8Li2Mg15	CEF (ST3)	(8)(2)(15)	(Cu)(Li)(Mg)
Cu8Zr3	CEF (ST2)	(8)(3)	(Cu)(Zr)
Cu9Er2	CEF (ST2)	(0.8182)	(Cu)(Er)

Name	Model	Lattice Size	Constituent
		(0.1818)	
Cu9Mg2Y_t1	CEF (ST3)	(9)(2)(1)	(Cu)(Mg)(Y)
CuEr	CEF (ST2)	(0.5)(0.5)	(Cu)(Er)
CuMg2	CEF (SLN)	(1)(2)	(Cu,Ni)(Mg)
CuMg4Y_t9	CEF (ST3)	(1)(4)(1)	(Cu)(Mg)(Y)
CuMgY_t4	CEF (ST3)	(1)(1)(1)	(Cu)(Mg)(Y)
CuO	CEF (ST2)	(1)(1)	(Cu)(O)
CuSm	CEF (ST2)	(0.5)(0.5)	(Cu)(Sm)
CuSr	CEF (ST2)	(0.5)(0.5)	(Cu)(Sr)
CuZn_Al_gam2	CEF (SLN)	(4)(6)(16)	(Cu)(Cu,Zn)(Ag,Al,Cu,Mn,Zn)
CuZn_eps	CEF (SLN)	(1)	(Al,Cu,Zn)
CuZr2	CEF (ST2)	(1)(2)	(Cu)(Zr)
Cub	CEF (SLN)	(1)(1)	(Ag,Al,Ce,Co,Cu,Fe,Mg,Mn,Ni,Si,Sn,Zn)(Va)
Dhcp	CEF (SLN)	(1)	(Al,Ca,Ce,La,Mg,Nd,Pr,Sc,Y)
Dy2O3	CEF (ST2)	(2)(3)	(Dy)(O)
Er13Zn58	CEF (ST2)	(13)(58)	(Er)(Zn)
Er2Fe17	CEF (ST2)	(2)(17)	(Er)(Fe)
Er2Zn17_T1	CEF (ST2)	(2)(17)	(Er)(Zn)
Er2Zn17_T2	CEF (ST2)	(2)(17)	(Er)(Zn)

Name	Model	Lattice Size	Constituent
Er5Sb3	CEF (ST2)	(5)(3)	(Er)(Sb)
Er5Si3	CEF (ST2)	(5)(3)	(Er)(Si)
Er5Si4	CEF (ST2)	(5)(4)	(Er)(Si)
Er6Fe23	CEF (ST2)	(6)(23)	(Er)(Fe)
ErFe2	CEF (ST2)	(1)(2)	(Er)(Fe)
ErFe3	CEF (ST2)	(1)(3)	(Er)(Fe)
ErSb2	CEF (ST2)	(1)(2)	(Er)(Sb)
ErSb_T1	CEF (ST2)	(1)(1)	(Er)(Sb)
ErSb_T2	CEF (ST2)	(1)(1)	(Er)(Sb)
ErSi2_T1	CEF (ST2)	(1)(1.67)	(Er)(Si)
ErSi2_T2	CEF (ST2)	(1)(1.67)	(Er)(Si)
ErSi_T1	CEF (ST2)	(1)(1)	(Er)(Si)
ErSi_T2	CEF (ST2)	(1)(1)	(Er)(Si)
ErSix	CEF (ST2)	(1)(0.96)	(Er)(Si)
ErZn	CEF (ST2)	(1)(1)	(Er)(Zn)
ErZn12	CEF (ST2)	(1)(12)	(Er)(Zn)
ErZn2	CEF (ST2)	(1)(2)	(Er)(Zn)
ErZn3	CEF (ST2)	(1)(3)	(Er)(Zn)
ErZn5	CEF (ST2)	(1)(5)	(Er)(Zn)
Fcc	CEF (SLN)	(1)(1)	(Ag,Al,Bi,Ca,Ce,Co,Cu,Er,Fe,

Name	Model	Lattice Size	Constituent
			Gd,La,Li,Mg,Mn,Nd,Ni,P,Sb,Sc,Si,Sm,Sn,Sr,Y,Zn,Zr)(Va)
Fe17Sm2	CEF (ST2)	(0.894737) (0.105263)	(Fe)(Sm)
Fe17Y2	CEF (ST2)	(17)(2)	(Fe)(Y)
Fe23Y6	CEF (ST2)	(23)(6)	(Fe)(Y)
Fe23Zr6	CEF (ST2)	(0.793) (0.207)	(Fe)(Zr)
Fe2O3	CEF (ST2)	(2)(3)	(Fe)(O)
Fe2Sc_T1	CEF (ST2)	(2)(1)	(Fe)(Sc)
Fe2Sc_T2	CEF (ST2)	(2)(1)	(Fe)(Sc)
Fe2Sc_T3	CEF (ST2)	(9)(5)	(Fe)(Sc)
Fe2Si	CEF (ST2)	(2)(1)	(Fe)(Si)
Fe2Sm	CEF (ST2)	(0.666667) (0.333333)	(Fe)(Sm)
Fe2Y	CEF (ST2)	(2)(1)	(Fe)(Y)
Fe2Zr_C15	CEF (SLN)	(2)(1)	(Fe,Zr)(Fe,Zr)
Fe3O4	CEF (ST2)	(3)(4)	(Fe)(O)
Fe3Sm	CEF (ST2)	(0.75)(0.25)	(Fe)(Sm)
Fe3Sn2	CEF (ST2)	(3)(2)	(Fe)(Sn)
Fe3Y	CEF (ST2)	(3)(1)	(Fe)(Y)

Name	Model	Lattice Size	Constituent
Fe5Sn3	CEF (ST2)	(5)(3)	(Fe)(Sn)
Fe6Sc29	CEF (ST2)	(6)(29)	(Fe)(Sc)
FeNi_L12	CEF (SLN)	(0.25)(0.25) (0.25)(0.25) (1)	(Fe,Ni)(Fe,Ni)(Fe,Ni)(Fe,Ni)(Va)
FeO	CEF (ST2)	(1)(1)	(Fe)(O)
FeSb	CEF (SLN)	(0.3333) (0.3333) (0.3333)	(Sb)(Fe,Va)(Fe,Va)
FeSb2	CEF (ST2)	(0.3333) (0.6667)	(Fe)(Sb)
FeSi2_T1	CEF (SLN)	(1)(2)	(Fe)(Al,Si)
FeSi2_T2	CEF (SLN)	(3)(7)	(Fe)(Al,Mg,Si)
FeSn	CEF (ST2)	(1)(1)	(Fe)(Sn)
FeSn2	CEF (ST2)	(1)(2)	(Fe)(Sn)
FeZn	CEF (SLN)	(0.125) (0.875)	(Fe,Zn)(Fe,Zn)
FeZn_gam1	CEF (SLN)	(0.3)(0.7)	(Fe,Zn)(Fe,Zn)
FeZn_gam2	CEF (SLN)	(0.25)(0.75)	(Fe,Zn)(Fe,Zn)
FeZn_zeta	CEF (SLN)	(0.072) (0.928)	(Fe,Zn)(Fe,Zn)
FeZr2	CEF (SLN)	(1)(2)	(Fe,Zr)(Fe,Zr)

Name	Model	Lattice Size	Constituent
FeZr3	CEF (SLN)	(1)(3)	(Fe,Zr)(Fe,Zr)
Gas	GAS	(1)	(Ag,Al,Al2,Bi,Bi2,C,C2,C3,C4,C5,Ca,Ce,Co,Cu,Cu2,Dy,Er,Fe,Gd,La,Li,Li2,Mg,Mg2,Mn,Nd,Ni,P,P2,P4,Pr,Sb,Sb2,Sc,Sc2,Se,Se2,Se3,Se4,Se5,Se6,Se7,Se8,Si,Si2,Si3,Si4,Sm,Sn,Sr,Y,Zn,Zr,AlC,CSi,CSi2,C2Si,Li3C,Li4C,Li6C,O,O2,O3,Al2O,Al2O2,Al2O3,AlO,AlO2,C2O,C3O2,C1O1,C1O2,CaO,CeO,CuO,FeO,La2O,La2O2,LaO,Li2O,Li2O2,LiO,MgO,NdO,NdO2,NiO,PrO,ScO,SeO,SeO2,SiO,SiO2,Sn2O2,Sn3O3,Sn4O4,SnO,SnO2,Sr2O,SrO,YO,ZrO,ZrO2)
Gd10Al21Cu9	CEF (ST3)	(0.525)(0.225)(0.25)	(Al)(Cu)(Gd)
Gd10Al44Cu66	CEF (ST3)	(0.366667)(0.55)(0.083333)	(Al)(Cu)(Gd)
Gd11Mg24Zn64_H1	CEF (ST3)	(11)(24)(64)	(Gd)(Mg)(Zn)
Gd14Ag51	CEF (ST2)	(0.784615)(0.215385)	(Ag)(Gd)
Gd15Mg15Zn70_	CEF (ST3)	(15)(15)(70)	(Gd)(Mg)(Zn)

Name	Model	Lattice Size	Constituent
H2			
Gd16Sb39	CEF (ST2)	(16)(39)	(Gd)(Sb)
Gd20Mg19Zn81_F	CEF (ST3)	(20)(19)(81)	(Gd)(Mg)(Zn)
Gd2AlCu17	CEF (SLN)	(0.894737) (0.105263)	(Al,Cu)(Gd)
Gd2Cu9	CEF (ST2)	(0.818182) (0.181818)	(Cu)(Gd)
Gd2Fe17_T1	CEF (ST2)	(17)(2)	(Fe)(Gd)
Gd2Fe17_T2	CEF (ST2)	(17)(2)	(Fe)(Gd)
Gd2O3	CEF (ST2)	(2)(3)	(Gd)(O)
Gd30Al89Cu21	CEF (ST3)	(0.635714) (0.15) (0.214286)	(Al)(Cu)(Gd)
Gd3Al2	CEF (ST2)	(0.4)(0.6)	(Al)(Gd)
Gd3Ni2	CEF (ST2)	(3)(2)	(Gd)(Ni)
Gd4Sb3	CEF (ST2)	(4)(3)	(Gd)(Sb)
Gd5Al16Cu39	CEF (ST3)	(0.266667) (0.65) (0.083333)	(Al)(Cu)(Gd)
Gd5Sb3	CEF (ST2)	(0.625) (0.375)	(Gd)(Sb)
Gd5Si4	CEF (ST2)	(0.555556) (0.444444)	(Gd)(Si)

Name	Model	Lattice Size	Constituent
Gd6Fe23	CEF (ST2)	(23)(6)	(Fe)(Gd)
Gd6Mn23	CEF (SLN)	(23)(6)	(Mg,Mn)(Gd)
GdAg	CEF (ST2)	(0.5)(0.5)	(Ag)(Gd)
GdAg2	CEF (ST2)	(0.666667) (0.333333)	(Ag)(Gd)
GdAgMg11_X	CEF (SLN)	(0.15)(0.85)	(Ag,Gd)(Mg)
GdAl	CEF (ST2)	(0.5)(0.5)	(Al)(Gd)
GdAl4Mg_C14	CEF (ST3)	(0.666667) (0.166667) (0.166667)	(Al)(Gd)(Mg)
GdAl8Cu4	CEF (ST3)	(0.615385) (0.307692) (0.076923)	(Al)(Cu)(Gd)
GdAlCu	CEF (ST3)	(0.333333) (0.333333) (0.333334)	(Al)(Cu)(Gd)
GdCu5	CEF (ST2)	(0.833333) (0.166667)	(Cu)(Gd)
GdFe2_C15	CEF (ST2)	(2)(1)	(Fe)(Gd)
GdFe3	CEF (ST2)	(3)(1)	(Fe)(Gd)
GdMg2_C15L	CEF (SLN)	(0.333333) (0.666667)	(Gd,Mg,Y)(Gd,Li,Mg,Zn)
GdMg3_DO19	CEF (SLN)	(0.75)(0.25)	(Gd,Mg)(Gd,Mg)(Va)

Name	Model	Lattice Size	Constituent
		(0.5)	
GdMg7	CEF (SLN)	(0.875) (0.125)(0.5)	(Gd,Mg)(Gd,Mg)(Va)
GdMn12	CEF (ST2)	(12)(1)	(Mn)(Gd)
GdMn2_C15	CEF (SLN)	(2)(1)	(Mg,Mn)(Gd)
GdNi4	CEF (ST2)	(1)(4)	(Gd)(Ni)
GdSb_T1	CEF (ST2)	(1)(1)	(Gd)(Sb)
GdSb_T2	CEF (ST2)	(1)(1)	(Gd)(Sb)
Halite	CEF (SLN)	(1)(1)	(Ca,Mg)(O)
Hcp	CEF (SLN)	(1)(0.5)	(Ag,Al,Bi,Ca,Ce,Co,Cu,Dy,Er,Fe, Gd,La,Li,Mg,Mn,Nd,Ni,O,Pr,Sb, Sc,Se,Si,Sm,Sn,Sr,Y,Zn,Zr)(Va)
La10Cu85Ni5	CEF (ST3)	(85)(10)(5)	(Cu)(La)(Ni)
La11Sn10	CEF (ST2)	(0.524) (0.476)	(La)(Sn)
La20Mg77Si3	CEF (ST3)	(0.2) (0.76667) (0.03333)	(La)(Mg)(Si)
La25Al66Mg9	CEF (ST3)	(66)(25)(9)	(Al)(La)(Mg)
La25Mg25Si50	CEF (ST3)	(0.25)(0.25) (0.5)	(La)(Mg)(Si)
La2Mg4Si4	CEF (ST3)	(0.2)(0.4)(0.4)	(La)(Mg)(Si)

Name	Model	Lattice Size	Constituent
La2Ni3	CEF (SLN)	(2)(3)	(La)(Ni,Cu)
La2Ni7_T2	CEF (ST2)	(7)(2)	(Ni)(La)
La2O3	CEF (ST2)	(2)(3)	(La)(O)
La2Sb	CEF (ST2)	(2)(1)	(La)(Sb)
La2Sn3	CEF (ST2)	(0.4)(0.6)	(La)(Sn)
La36Si64	CEF (SLN)	(0.36)(0.64)	(La)(Al,Si)
La3Al40Mg17	CEF (ST3)	(40)(3)(17)	(Al)(La)(Mg)
La3Al7	CEF (ST2)	(0.707) (0.293)	(Al)(La)
La3Cu37	CEF (ST2)	(37)(3)	(Cu)(La)
La3Sb2	CEF (ST2)	(3)(2)	(La)(Sb)
La3Sn5	CEF (ST2)	(0.375) (0.625)	(La)(Sn)
La4Mg2Si4	CEF (SLN)	(0.6)(0.4)	(La,Mg)(Si)
La5Mg42Zn53	CEF (ST3)	(0.05)(0.42) (0.53)	(La)(Mg)(Zn)
La5Sn3_T1	CEF (ST2)	(0.625) (0.375)	(La)(Sn)
La5Sn3_T2	CEF (ST2)	(0.625) (0.375)	(La)(Sn)
La5Sn4	CEF (ST2)	(0.555) (0.445)	(La)(Sn)

Name	Model	Lattice Size	Constituent
La7Ni16	CEF (SLN)	(7)(16)	(La)(Ni,Cu)
La82Mg167Si_C15	CEF (ST3)	(0.3293) (0.6667) (0.004)	(La)(Mg)(Si)
LaSb	CEF (ST2)	(1)(1)	(La)(Sb)
LaSb2	CEF (ST2)	(1)(2)	(La)(Sb)
LaSn	CEF (ST2)	(0.5)(0.5)	(La)(Sn)
LaSn3	CEF (ST2)	(0.25)(0.75)	(La)(Sn)
LaZn13	CEF (ST2)	(0.071) (0.929)	(La)(Zn)
LaZn4	CEF (ST2)	(0.2)(0.8)	(La)(Zn)
Li12Mg3Si4	CEF (ST3)	(0.631579) (0.157895) (0.210526)	(Li)(Mg)(Si)
Li12Si7	CEF (ST2)	(12)(7)	(Li)(Si)
Li13Si4	CEF (ST2)	(13)(4)	(Li)(Si)
Li13Sn5	CEF (ST2)	(0.722222) (0.277778)	(Li)(Sn)
Li15Si4	CEF (ST2)	(15)(4)	(Li)(Si)
Li16Si4	CEF (ST2)	(16.42)(4)	(Li)(Si)
Li17Si4	CEF (ST2)	(17)(4)	(Li)(Si)
Li17Sn4	CEF (ST2)	(0.809524)	(Li)(Sn)

Name	Model	Lattice Size	Constituent
		(0.190476)	
Li2C2_T1	CEF (ST2)	(0.5)(0.5)	(C)(Li)
Li2C2_T2	CEF (ST2)	(0.5)(0.5)	(C)(Li)
Li2MgSi	CEF (ST3)	(0.5)(0.25) (0.25)	(Li)(Mg)(Si)
Li2O	CEF (ST2)	(2)(1)	(Li)(O)
Li2O2	CEF (ST2)	(2)(2)	(Li)(O)
Li2Sn5	CEF (ST2)	(0.285714) (0.714286)	(Li)(Sn)
Li2Zn3	CEF (ST2)	(0.4)(0.6)	(Li)(Zn)
Li2Zn5	CEF (ST2)	(0.285715) (0.714285)	(Li)(Zn)
Li5Sn2	CEF (ST2)	(0.714286) (0.285714)	(Li)(Sn)
Li7Si3	CEF (ST2)	(7)(3)	(Li)(Si)
Li7Sn2	CEF (SLN)	(0.777778) (0.222222)	(Li,Sn)(Sn)
Li7Sn3	CEF (ST2)	(0.7)(0.3)	(Li)(Sn)
Li8MgSi6	CEF (ST3)	(0.533333) (0.066667) (0.4)	(Li)(Mg)(Si)
LiC6	CEF (ST2)	(6)(1)	(C)(Li)

Name	Model	Lattice Size	Constituent
LiSi	CEF (ST2)	(1)(1)	(Li)(Si)
LiSn	CEF (ST2)	(0.5)(0.5)	(Li)(Sn)
LiZn4	CEF (ST2)	(0.2)(0.8)	(Li)(Zn)
Liquid	CEF (SLN)	(1)	(Ag,Al,Bi,Bi2Mg3,C,Ca,Ca2Sn,CaO,Ce,Co,Cu,Dy,Er,Fe,Gd,La,LaSn,Li,Li2C2,Li4Sn,Mg,Mg2Sn,MgO,Mn,O,P,Nd,Ni,Pr,Sb,Sc,Se,Si,Sm,Sn,Sr,Y,Zn,Zr)
Mg17Sr2	CEF (SLN)	(17)(2)	(Al,Mg)(Ca,Sr)
Mg23Sr6	CEF (SLN)	(23)(6)	(Al,Mg)(Sr)
Mg28Y7Zn65_Z	CEF (SLN)	(28)(7)(65)	(Mg)(Y)(Mg,Zn)
Mg2C3	CEF (ST2)	(2)(3)	(Mg)(C)
Mg2M	CEF (SLN)	(0.5)(0.25)(0.25)	(Bi,Mg)(Bi,Sn,Si)(Li,Va)
Mg2Ni	CEF (SLN)	(2)(1)	(Mg)(Cu,Ni)
Mg2Sm	CEF (ST2)	(2)(1)	(Mg)(Sm)
Mg2Zn11	CEF (SLN)	(5)(6)(2)	(Al,Zn)(Cu,Zn)(Mg)
Mg2Zn3	CEF (SLN)	(2)(3)	(Mg)(Al,Cu,Zn)
Mg38Sr9	CEF (SLN)	(38)(9)	(Al,Mg)(Ca,Sr)
Mg3P2	CEF (ST2)	(3)(2)	(Mg)(P)
Mg3Sb2_T1	CEF (SLN)	(0.6)(0.4)	(Mg)(Mg,Sb)

Name	Model	Lattice Size	Constituent
Mg3Sb2_T2	CEF (SLN)	(0.4)(0.5)(0.1)	(Mg,Sb)(Mg,Sb)(Mg)
Mg3Sm	CEF (ST2)	(3)(1)	(Mg)(Sm)
Mg41Sm5	CEF (ST2)	(41)(5)	(Mg)(Sm)
Mg47Y8Zn6_10H	CEF (ST3)	(47)(8)(6)	(Mg)(Y)(Zn)
Mg59Y8Zn6_18R	CEF (SLN)	(59)(6)(2)	(Mg)(Mg2,YZn)(Mg,Y)
Mg5Sm	CEF (ST2)	(5)(1)	(Mg)(Sm)
Mg5Zn2	CEF (SLN)	(51)(20)	(Mg)(Mn,Zn)
Mg65Y20Zn15	CEF (ST3)	(65)(20)(15)	(Mg)(Y)(Zn)
Mg71R8Zn6_14H	CEF (SLN)	(71)(6)(2)	(Mg)(Mg2,GdZn,YZn)(Mg,Gd,Y)
MgC2	CEF (ST2)	(1)(2)	(Mg)(C)
MgNi2_C36	CEF (SLN)	(1)(2)	(Al,Cu,Mg,Ni,Si,Zn) (Al,Cu,Mg,Ni,Si,Zn)
MgSc	CEF (ST2)	(0.5)(0.5)	(Mg)(Sc)
MgSe	CEF (ST2)	(1)(1)	(Mg)(Se)
MgZn	CEF (SLN)	(12)(13)	(Mg)(Al,Cu,Zn)
MgZn2_C14	CEF (SLN)	(1)(2)	(Al,Cu,Mg,Mn,Ni,Si,Zn) (Al,Co,Cu,Li,Mg,Mn,Ni,Si,Zn)
Mn11Si19	CEF (SLN)	(0.146)(0.22) (0.244)(0.39)	(Mn)(Mn,Va)(Mn,Si)(Si)
Mn12Y	CEF (ST2)	(12)(1)	(Mn)(Y)
Mn19Sn6	CEF (ST2)	(19)(6)	(Mn)(Sn)

Name	Model	Lattice Size	Constituent
Mn23Sm6	CEF (ST2)	(0.793) (0.207)	(Mn)(Sm)
Mn23Y6	CEF (SLN)	(23)(6)	(Mg,Mn)(Y)
Mn2M_C14	CEF (SLN)	(2)(1)	(Mn)(Sc,Zr,Va)
Mn2Ni	CEF (ST2)	(2)(1)	(Mn)(Ni)
Mn2O3	CEF (ST2)	(2)(3)	(Mn)(O)
Mn2Sm	CEF (ST2)	(0.667) (0.333)	(Mn)(Sm)
Mn2Sn	CEF (ST2)	(2)(1)	(Mn)(Sn)
Mn2Y_C15	CEF (SLN)	(2)(1)	(Mg,Mn)(Y)
Mn2Zn3_eps	CEF (SLN)	(1)	(Mn,Zn)
Mn3O4	CEF (ST2)	(3)(4)	(Mn)(O)
Mn3Si	CEF (SLN)	(3)(1)	(Fe,Mn)(Si)
Mn5Si3	CEF (SLN)	(5)(3)	(Fe,Mn)(Si)
Mn5Zn21	CEF (SLN)	(154)(154) (231)(461)	(Mn,Zn)(Mn,Zn)(Mn,Zn)(Zn)
Mn6Si	CEF (SLN)	(0.49)(0.36) (0.15)	(Mn)(Mn,Si)(Mn,Si,Va)
Mn8Sc2	CEF (ST2)	(0.7931) (0.2069)	(Mn)(Sc)
Mn9Si2	CEF (SLN)	(0.613) (0.215)	(Mn)(Mn,Si)(Mn,Si)(Si)

Name	Model	Lattice Size	Constituent
		(0.108) (0.064)	
MnNi	CEF (ST2)	(1)(1)	(Mn)(Ni)
MnNi2	CEF (ST2)	(1)(2)	(Mn)(Ni)
MnO	CEF (ST2)	(1)(1)	(Mn)(O)
MnO2	CEF (ST2)	(1)(2)	(Mn)(O)
MnSc4	CEF (ST2)	(0.2)(0.8)	(Mn)(Sc)
MnSi	CEF (SLN)	(1)(1)	(Fe,Mn)(Mg,Si)
MnSn2	CEF (ST2)	(1)(2)	(Mn)(Sn)
MnZn	CEF (ST2)	(1)(1)	(Mn)(Zn)
MnZn13	CEF (SLN)	(9)(107)(9)	(Mn,Va)(Zn)(Mn,Zn)
MnZn3	CEF (SLN)	(3)(1)	(Mn,Zn)(Mn,Zn)
MnZn9_T1	CEF (SLN)	(58)(180) (525)(237)	(Mn)(Mg,Mn,Zn)(Zn)(Zn)
MnZn9_T2	CEF (SLN)	(9)(1)	(Mn,Zn)(Mn,Zn)
Nd14Ag51	CEF (ST2)	(0.784615) (0.215385)	(Ag)(Nd)
Nd15Mg30Zn55_ tau3	CEF (ST3)	(0.3)(0.15) (0.55)	(Mg)(Nd)(Zn)
Nd2Fe17	CEF (ST2)	(17)(2)	(Fe)(Nd)
Nd2O3	CEF (ST2)	(2)(3)	(Nd)(O)

Name	Model	Lattice Size	Constituent
Nd2Y	CEF (SLN)	(2)(1)	(Nd,Y)(Nd,Y)
Nd5Fe17	CEF (ST2)	(17)(5)	(Fe)(Nd)
Nd5Mg35Zn60_tau1	CEF (ST3)	(0.35)(0.05)(0.6)	(Mg)(Nd)(Zn)
Nd6Mn23	CEF (ST2)	(23)(6)	(Mn)(Nd)
NdAg	CEF (ST2)	(0.5)(0.5)	(Ag)(Nd)
NdAg2	CEF (ST2)	(0.666667)(0.333333)	(Ag)(Nd)
NdAgMg11	CEF (ST3)	(1)(1)(11)	(Nd)(Ag)(Mg)
NdAl	CEF (SLN)	(1)(1)	(Al)(Ce,Nd)
NdAl3Cu	CEF (ST3)	(3)(1)(1)	(Al)(Cu)(Nd)
NdAl8Cu4	CEF (ST3)	(8)(4)(1)	(Al)(Cu)(Nd)
NdMgZn_tau2	CEF (SLN)	(0.92)(0.08)	(Mg,Zn)(Nd)
NdMn2_C14	CEF (ST2)	(2)(1)	(Mn)(Nd)
Ni10Zr7	CEF (ST2)	(10)(7)	(Ni)(Zr)
Ni11Zr9	CEF (ST2)	(11)(9)	(Ni)(Zr)
Ni17Sm2	CEF (ST2)	(17)(2)	(Ni)(Sm)
Ni17Y2	CEF (ST2)	(17)(2)	(Ni)(Y)
Ni19Sm5	CEF (ST2)	(19)(5)	(Ni)(Sm)
Ni21Zr8	CEF (ST2)	(21)(8)	(Ni)(Zr)
Ni2Sc	CEF (SLN)	(0.6667)	(Ni,Sc)(Ni,Sc)

Name	Model	Lattice Size	Constituent
		(0.3333)	
Ni2Si_T1	CEF (ST2)	(2)(1)	(Ni)(Si)
Ni2Si_T2	CEF (SLN)	(2)(1)	(Ni,Si)(Si)
Ni2Sm	CEF (ST2)	(2)(1)	(Ni)(Sm)
Ni2Y3	CEF (ST2)	(2)(3)	(Ni)(Y)
Ni2Y_C15	CEF (ST2)	(2)(1)	(Ni)(Y)
Ni2Zn15	CEF (ST2)	(2)(15)	(Ni)(Zn)
Ni31Si12	CEF (ST2)	(31)(12)	(Ni)(Si)
Ni3Sb	CEF (SLN)	(0.25)(0.5) (0.25)	(Sb)(Ni,Va)(Ni,Va)
Ni3Sb_delta	CEF (SLN)	(0.75)(0.25)	(Ni)(Ni,Sb)
Ni3Si2	CEF (ST2)	(3)(2)	(Ni)(Si)
Ni3Si_T1	CEF (ST2)	(19)(6)	(Ni)(Si)
Ni3Si_T2	CEF (ST2)	(149)(51)	(Ni)(Si)
Ni3Sm	CEF (ST2)	(3)(1)	(Ni)(Sm)
Ni3Sn2_T1	CEF (SLN)	(0.2)(0.4)(0.4)	(Sn)(Ni,Sn)(Ni)
Ni3Sn2_T2	CEF (SLN)	(0.33333) (0.33334) (0.33333)	(Ni)(Ni,Sn)(Sn)
Ni3Sn4	CEF (SLN)	(0.25)(0.25) (0.5)	(Ni)(Ni,Sn)(Sn)

Name	Model	Lattice Size	Constituent
Ni3Sn_T1	CEF (ST2)	(0.75)(0.25)	(Ni)(Sn)
Ni3Sn_T2	CEF (SLN)	(0.25)(0.25) (0.5)	(Ni,Sn)(Ni,Sn)(Ni)
Ni3Y	CEF (ST2)	(3)(1)	(Ni)(Y)
Ni3Zr	CEF (ST2)	(3)(1)	(Ni)(Zr)
Ni4Y	CEF (ST2)	(4)(1)	(Ni)(Y)
Ni5Sb2	CEF (SLN)	(0.7143) (0.2857)	(Ni)(Ni,Sb)
Ni5Sc	CEF (ST2)	(0.833) (0.167)	(Ni)(Sc)
Ni5Sm	CEF (ST2)	(5)(1)	(Ni)(Sm)
Ni5Y	CEF (ST2)	(5)(1)	(Ni)(Y)
Ni5Zr	CEF (SLN)	(5)(1)	(Ni,Zr)(Zr,Va)
Ni7Sc2	CEF (ST2)	(0.778) (0.222)	(Ni)(Sc)
Ni7Sm2	CEF (ST2)	(7)(2)	(Ni)(Sm)
Ni7Y2	CEF (ST2)	(7)(2)	(Ni)(Y)
Ni7Zr2	CEF (ST2)	(7)(2)	(Ni)(Zr)
NiO	CEF (ST2)	(1)(1)	(Ni)(O)
NiSb	CEF (SLN)	(0.3333) (0.3333) (0.3333)	(Sb)(Ni,Va)(Ni,Va)

Name	Model	Lattice Size	Constituent
NiSb2	CEF (ST2)	(0.3333) (0.6667)	(Ni)(Sb)
NiSc	CEF (ST2)	(0.47)(0.53)	(Ni)(Sc)
NiSc2	CEF (ST2)	(0.28)(0.72)	(Ni)(Sc)
NiSi	CEF (ST2)	(1)(1)	(Ni)(Si)
NiSi2	CEF (ST2)	(1)(2)	(Ni)(Si)
NiSm	CEF (ST2)	(1)(1)	(Ni)(Sm)
NiSm3	CEF (ST2)	(1)(3)	(Ni)(Sm)
NiSr	CEF (ST2)	(1)(1)	(Ni)(Sr)
NiY	CEF (ST2)	(1)(1)	(Ni)(Y)
NiY3	CEF (ST2)	(1)(3)	(Ni)(Y)
NiZn_T1	CEF (SLN)	(1)(1)	(Ni,Zn)(Ni,Zn)
NiZn_T2	CEF (SLN)	(1)(1)	(Ni,Zn)(Ni,Zn)
NiZn_gam	CEF (SLN)	(4)(4)(18)	(Ni,Zn)(Ni)(Zn)
NiZr	CEF (ST2)	(1)(1)	(Ni)(Zr)
NiZr2	CEF (ST2)	(1)(2)	(Ni)(Zr)
P_red	CEF (ST1)	(1)	(P)
P_white	CEF (ST1)	(1)	(P)
Pr2O3	CEF (ST2)	(2)(3)	(Pr)(O)
Pr2Sb	CEF (ST2)	(0.66667) (0.33333)	(Pr)(Sb)

Name	Model	Lattice Size	Constituent
Pr4Sb3	CEF (ST2)	(0.57143) (0.42857)	(Pr)(Sb)
Pr5Sb3	CEF (ST2)	(0.625) (0.375)	(Pr)(Sb)
Pr6O11	CEF (ST2)	(6)(11)	(Pr)(O)
Pr7O12	CEF (ST2)	(7)(12)	(Pr)(O)
PrO2	CEF (ST2)	(1)(2)	(Pr)(O)
PrSb	CEF (ST2)	(0.5)(0.5)	(Pr)(Sb)
PrSb2	CEF (ST2)	(0.33333) (0.66667)	(Pr)(Sb)
R13Zn58	CEF (SLN)	(0.183) (0.817)	(Ce,Gd,Nd,Y)(Zn)
R2Al	CEF (SLN)	(1)(2)	(Al)(Ce,Gd,Nd,Y)
R2Cu7	CEF (SLN)	(0.777778) (0.222222)	(Cu)(Gd,Y,Zr)
R2Ni17	CEF (SLN)	(2)(17)	(Gd,Nd)(Ni)
R2Ni7_T1	CEF (SLN)	(2)(7)	(Ce,Gd,La,Nd)(Cu,Ni)
R2Zn17	CEF (SLN)	(2)(17)	(Ce,La,Gd,Nd,Y)(Mg,Zn)
R3Al11_T1	CEF (SLN)	(11)(3)	(Al)(Ce,La,Nd)
R3Al11_T2	CEF (SLN)	(11)(3)	(Al)(Ce,La,Nd)
R3Al_T1	CEF (SLN)	(1)(3)	(Al)(Ce,La,Nd)

Name	Model	Lattice Size	Constituent
R3Al_T2	CEF (ST2)	(1)(3)	(Al)(Ce)
R3Ni	CEF (SLN)	(3)(1)	(Gd,La,Nd)(Ni)
R3Si2	CEF (SLN)	(0.6)(0.4)	(Ce,La,Mg)(Si)
R3Si5	CEF (SLN)	(0.375) (0.625)	(Ce,Gd)(Si)
R3Zn11	CEF (SLN)	(0.214) (0.786)	(Ce,Gd,Nd,Y)(Zn)
R3Zn22	CEF (SLN)	(0.12)(0.88)	(Ce,Gd,La,Nd)(Zn)
R5Mg24	CEF (SLN)	(24)(5)	(Mg)(Ce,Dy,Er,Gd,Mg,Y,Zn)
R5Mg41	CEF (SLN)	(5)(41)	(Ca,Ce,La,Nd,Pr,Y)(Mg,Zn)
R5Si3_T1	CEF (SLN)	(0.625) (0.375)	(Gd,Y)(Si)
R5Si3_T2	CEF (SLN)	(0.625) (0.375)	(Ce,La)(Si)
R5Si4	CEF (SLN)	(0.555556) (0.444444)	(Ce,La,Mg)(Si)
R7Ni3	CEF (SLN)	(7)(3)	(Ce,La,Nd)(Ni)
RAl	CEF (SLN)	(1)(1)	(Al)(Ce,La,Nd)
RAl3	CEF (SLN)	(0.75)(0.25)	(Al)(Ce,La,Gd,Nd,Y)
RCu2	CEF (SLN)	(0.666667) (0.333333)	(Al,Cu,Ni)(Ce,La,Gd,Nd,Sc,Y)
RCu4	CEF (SLN)	(0.8)(0.2)	(Cu)(Ce,La,Nd,Sc,Y,Zr)

Name	Model	Lattice Size	Constituent
RCu6_T1	CEF (SLN)	(0.857143) (0.142857)	(Cu)(La,Gd)
RCu6_T2	CEF (SLN)	(0.857143) (0.142857)	(Cu)(Ce,La,Gd,Nd)
RCu_T1	CEF (SLN)	(0.5)(0.5)	(Ce,La,Nd)(Cu,Ni)
RCu_T2	CEF (SLN)	(0.5)(0.5)	(Cu)(Gd,Sc,Y,Zr)
RM3_W	CEF (SLN)	(0.25)(0.25) (0.5)	(Mg)(Gd,Y)(Mg,Zn)
RMg12	CEF (SLN)	(1)(12)	(Ce,La,Nd,Pr,Y)(Al,Mg,Zn)
RMg2_C14L	CEF (SLN)	(1)(2)	(Ce,Er,Dy,Gd,Nd,Mg,Y) (Er,Dy,Mg,Y)
RMg2_C15	CEF (SLN)	(0.666667) (0.333333)	(Al,Cu,Mg,Zn) (Ce,Gd,La,Nd,Pr,Y)
RMg3	CEF (SLN)	(1)(3)	(Ce,Dy,Gd,La,Mg,Nd,Pr,Y) (Gd,Li,Mg,Zn)
RMg3Zn6_I	CEF (SLN)	(1)(3)(6)	(Gd,Y)(Mg)(Mg,Zn)
RMg5	CEF (SLN)	(5)(1)	(Mg,Zn)(Ag,Ce,Gd,Mg,Nd,Y)
RMg_B2	CEF (SLN)	(0.5)(0.5)	(Ce,Dy,Gd,La,Mg,Nd,Pr,Y,Zn) (Al,Mg,Mn,Li,Zn)
RNi	CEF (SLN)	(1)(1)	(Ce,Gd,La,Nd)(Cu,Ni)
RNi2_C15	CEF (SLN)	(1)(2)	(Ce,Ni,Gd,Nd)(Ce,Ni)
RNi3	CEF (SLN)	(1)(3)	(Ce,Gd,La,Nd)(Cu,Ni)

Name	Model	Lattice Size	Constituent
RSi	CEF (SLN)	(0.5)(0.5)	(Ce,Gd,La)(Si)
RSi2_T1	CEF (SLN)	(0.333333) (0.666667)	(Gd,Y)(Si)
RSi2_T2	CEF (SLN)	(0.333333) (0.666667)	(Ce,La,Y)(Al,Si)
RZn11	CEF (SLN)	(0.083) (0.917)	(Ce,La,Nd)(Zn)
RZn12	CEF (SLN)	(1)(12)	(Gd,Y)(Zn)
RZn2	CEF (SLN)	(0.333333) (0.666667)	(Ce,Gd,La,Nd)(Zn)
RZn3	CEF (SLN)	(1)(3)	(Ce,Gd,Nd,Y)(Zn)
RZn5	CEF (SLN)	(0.167) (0.833)	(Ce,La)(Zn)
Rhomb	CEF (SLN)	(1)	(Bi,Sb,Sn,Zn)
Rhomb_C19	CEF (SLN)	(1)	(Al,Gd,Mg,Sm)
Sb2Sm	CEF (ST2)	(0.333) (0.667)	(Sm)(Sb)
Sb2Sn3	CEF (ST2)	(2)(3)	(Sb)(Sn)
Sb2Zn3_T1	CEF (ST2)	(2)(3)	(Sb)(Zn)
Sb2Zn3_T2	CEF (ST2)	(2.025) (2.975)	(Sb)(Zn)
Sb3Sm4	CEF (ST2)	(0.571) (0.429)	(Sm)(Sb)

Name	Model	Lattice Size	Constituent
Sb3Sm5_T1	CEF (ST2)	(0.625) (0.375)	(Sm)(Sb)
Sb3Sm5_T2	CEF (ST2)	(0.625) (0.375)	(Sm)(Sb)
Sb3Zn4_T0	CEF (SLN)	(3)(4)	(Sb)(Zn,Va)
Sb3Zn4_T1	CEF (ST2)	(3.087) (3.913)	(Sb)(Zn)
Sb3Zn4_T2	CEF (ST2)	(3.094) (3.906)	(Sb)(Zn)
SbSm	CEF (ST2)	(0.5)(0.5)	(Sm)(Sb)
SbSn	CEF (SLN)	(1)	(Sb,Sn)
SbZn	CEF (SLN)	(1)(1)	(Sb)(Zn,Va)
Sc11Sn10	CEF (ST2)	(0.523) (0.477)	(Sc)(Sn)
Sc13Zn58	CEF (ST2)	(0.183099) (0.816901)	(Sc)(Zn)
Sc2O3	CEF (ST2)	(2)(3)	(Sc)(O)
Sc3Zn17	CEF (ST2)	(0.15)(0.85)	(Sc)(Zn)
Sc5Si3	CEF (ST2)	(5)(3)	(Sc)(Si)
Sc5Si4	CEF (ST2)	(5)(4)	(Sc)(Si)
Sc5Sn3_T1	CEF (ST2)	(0.625) (0.375)	(Sc)(Sn)

Name	Model	Lattice Size	Constituent
Sc5Sn3_T2	CEF (ST2)	(0.625) (0.375)	(Sc)(Sn)
Sc6Sn5	CEF (ST2)	(0.545) (0.455)	(Sc)(Sn)
ScSi	CEF (ST2)	(1)(1)	(Sc)(Si)
ScSix	CEF (ST2)	(1)(1.67)	(Sc)(Si)
ScSn2	CEF (ST2)	(0.333) (0.667)	(Sc)(Sn)
ScZn	CEF (ST2)	(0.5)(0.5)	(Sc)(Zn)
ScZn12	CEF (ST2)	(0.076923) (0.923077)	(Sc)(Zn)
ScZn2	CEF (ST2)	(0.333333) (0.666667)	(Sc)(Zn)
Se2O5	CEF (ST2)	(2)(5)	(Se)(O)
SeO2	CEF (ST2)	(1)(2)	(Se)(O)
SeO3	CEF (ST2)	(1)(3)	(Se)(O)
Se_A8	CEF (ST1)	(1)	(Se)
Si2Sr	CEF (ST2)	(0.333333) (0.666667)	(Sr)(Si)
Si2Zr	CEF (ST2)	(2)(1)	(Si)(Zr)
Si2Zr3	CEF (ST2)	(2)(3)	(Si)(Zr)
Si3Sr5	CEF (ST2)	(0.625)	(Sr)(Si)

Name	Model	Lattice Size	Constituent
		(0.375)	
Si3Zr5	CEF (ST2)	(3)(5)	(Si)(Zr)
Si4Y5	CEF (ST2)	(4)(5)	(Si)(Y)
Si4Zr5	CEF (ST2)	(4)(5)	(Si)(Zr)
Si5Y3_T1	CEF (ST2)	(5)(3)	(Si)(Y)
Si5Y3_T2	CEF (ST2)	(5)(3)	(Si)(Y)
SiC	CEF (ST2)	(1)(1)	(C)(Si)
SiO2_cris	CEF (ST2)	(1)(2)	(Si)(O)
SiO2_liq	CEF (ST2)	(1)	(SiO2)
SiO2_qtz	CEF (ST2)	(1)(2)	(Si)(O)
SiO2_trid	CEF (ST2)	(1)(2)	(Si)(O)
SiO_am	CEF (ST2)	(1)(1)	(Si)(O)
SiP	CEF (ST2)	(1)(1)	(P)(Si)
SiP2	CEF (ST2)	(2)(1)	(P)(Si)
SiSr	CEF (ST2)	(0.5)(0.5)	(Sr)(Si)
SiSr2	CEF (ST2)	(0.666667) (0.333333)	(Sr)(Si)
SiY	CEF (ST2)	(1)(1)	(Si)(Y)
SiZr	CEF (ST2)	(1)(1)	(Si)(Zr)
SiZr2	CEF (ST2)	(1)(2)	(Si)(Zr)

Name	Model	Lattice Size	Constituent
SiZr3	CEF (ST2)	(1)(3)	(Si)(Zr)
Si_diam	CEF (SLN)	(1)	(Al,C,Li,Mg,Mn,O,P,Sb,Si,Sn,Zn)
Sm11Sn10	CEF (ST2)	(0.524) (0.476)	(Sm)(Sn)
Sm13Zn58	CEF (ST2)	(0.1831) (0.8169)	(Sm)(Zn)
Sm2Sn3	CEF (ST2)	(0.4)(0.6)	(Sm)(Sn)
Sm2Zn17	CEF (ST2)	(0.1053) (0.8847)	(Sm)(Zn)
Sm3Zn11	CEF (ST2)	(0.2143) (0.7857)	(Sm)(Zn)
Sm3Zn22	CEF (ST2)	(0.12)(0.88)	(Sm)(Zn)
Sm4Sn3	CEF (ST2)	(0.571) (0.429)	(Sm)(Sn)
Sm5Sn3	CEF (ST2)	(0.625) (0.375)	(Sm)(Sn)
Sm5Sn4	CEF (ST2)	(0.556) (0.444)	(Sm)(Sn)
SmSn2	CEF (ST2)	(0.333) (0.667)	(Sm)(Sn)
SmSn3	CEF (ST2)	(0.25)(0.75)	(Sm)(Sn)
SmZn	CEF (ST2)	(0.5)(0.5)	(Sm)(Zn)
SmZn11	CEF (ST2)	(0.0769)	(Sm)(Zn)

Name	Model	Lattice Size	Constituent
		(0.9231)	
SmZn2	CEF (ST2)	(0.3333) (0.6667)	(Sm)(Zn)
SmZn3	CEF (ST2)	(0.25)(0.75)	(Sm)(Zn)
Sn10Y11	CEF (ST2)	(10)(11)	(Sn)(Y)
Sn2Y	CEF (ST2)	(2)(1)	(Sn)(Y)
Sn2Zr	CEF (ST2)	(2)(1)	(Sn)(Zr)
Sn3Sr	CEF (ST2)	(0.25)(0.75)	(Sr)(Sn)
Sn3Sr5	CEF (ST2)	(0.625) (0.375)	(Sr)(Sn)
Sn3Y	CEF (ST2)	(0.75)(0.25)	(Sn)(Y)
Sn3Y5	CEF (ST2)	(0.375) (0.625)	(Sn)(Y)
Sn3Zr5	CEF (ST2)	(3)(5)	(Sn)(Zr)
Sn4Sr	CEF (ST2)	(0.2)(0.8)	(Sr)(Sn)
Sn4Y5	CEF (ST2)	(4)(5)	(Sn)(Y)
Sn5Sr3	CEF (ST2)	(0.375) (0.625)	(Sr)(Sn)
Sn5Y2	CEF (ST2)	(5)(2)	(Sn)(Y)
SnO	CEF (ST2)	(1)(1)	(Sn)(O)
SnO2	CEF (ST2)	(1)(2)	(Sn)(O)

Name	Model	Lattice Size	Constituent
SnSr	CEF (ST2)	(0.5)(0.5)	(Sr)(Sn)
SnSr2	CEF (ST2)	(0.666667) (0.333333)	(Sr)(Sn)
SnZr4	CEF (ST2)	(1)(4)	(Sn)(Zr)
SrO	CEF (ST2)	(1)(1)	(Sr)(O)
SrO2	CEF (ST2)	(1)(2)	(Sr)(O)
SrZn	CEF (ST2)	(1)(1)	(Sr)(Zn)
SrZn5	CEF (ST2)	(1)(5)	(Sr)(Zn)
Y2O3	CEF (ST2)	(2)(3)	(Y)(O)
YZn2_T1	CEF (ST2)	(1)(2)	(Y)(Zn)
YZn2_T2	CEF (ST2)	(1)(2)	(Y)(Zn)
YZn5_H	CEF (SLN)	(1)(1.5)(3.5)	(Y)(Mg,Zn)(Zn)
Zn22Zr	CEF (ST2)	(0.956522) (0.0434783)	(Zn)(Zr)
Zn2Zr3	CEF (ST2)	(0.4)(0.6)	(Zn)(Zr)
Zn2Zr_C15	CEF (ST2)	(0.666667) (0.333333)	(Zn)(Zr)
Zn39Zr5	CEF (ST2)	(0.886364) (0.113636)	(Zn)(Zr)
Zn3Zr_T1	CEF (ST2)	(0.75)(0.25)	(Zn)(Zr)
Zn3Zr_T2	CEF (ST2)	(0.75)(0.25)	(Zn)(Zr)

Name	Model	Lattice Size	Constituent
ZnO	CEF (ST2)	(1)(1)	(Zn)(O)
ZnZr	CEF (ST2)	(0.5)(0.5)	(Zn)(Zr)
ZnZr2	CEF (ST2)	(0.333333) (0.666667)	(Zn)(Zr)
ZrO2	CEF (ST2)	(1)(2)	(Zr)(O)