Thermo-Calc Software

TCS Al-based Alloy Database (TCAL7)

Thermo-Calc Version 2020b

Technical Information

Contents

About the TCS Al-based Alloy Database (TCAL)

Current Database Version

TCS Al-based Alloy Database (TCAL) is thermodynamic database developed for aluminum-based alloys, including but not limited to, the industrial grades. In addition to thermodynamic data, it has properties data available for:

- molar volume with thermal expansion coefficients,
- electrical resistivity,
- thermal conductivity,
- viscosity of metallic liquids, and
- surface tension of metallic liquids.

Molar volume with thermal expansion coefficients properties data have been available since TCAL2. Electrical resistivity, thermal conductivity, viscosity of metallic liquids and surface tension of metallic liquids properties data are available starting with TCAL7.

The CALPHAD Method

The Thermo-Calc databases are developed with the CALPHAD approach based on various types of experimental data and theoretical values (e.g. those from first-principles calculations). It is based on the critical evaluation of binary, ternary and in some cases, important higher order systems which enables predictions to be made for multicomponent systems and alloys of industrial importance. Among these, the thermodynamic database is of fundamental importance.

CALPHAD is originally an abbreviation for *CALculation of PHAse Diagrams*, but was later expanded to refer to *computer coupling of phase diagrams and thermochemistry*. More about the CALPHAD methodology, including some of its history, is available on the Thermo-Calc Software website.

Use Case Examples

There are examples available to both demonstrate the *validation* of the database and to showcase the types of *calculations* that can be used for different materials or application areas such as process metallurgy, heat treatment, and more depending on the database. Sometimes an example is both a validation and a calculation example.

Some use case examples of how this database can be used include the following. Use it to:

- Calculate various phase diagrams and property diagrams in the assessed systems as well as to extrapolate higher-order systems, and predict phase formation, phase fractions and phase compositions in multicomponent aluminum alloys.
- Predict non-equilibrium solidification behavior of aluminum alloys. This can be at specific cooling rates when you take into account back diffusion using the Scheil calculation options in Thermo-Calc.
- Intetegrate with a compatible atomic mobility database and use it to simulate diffusion-controlled phase transformations with the add-on Diffusion Module (DICTRA) and multi-particle precipitation kinetics with the add-on Precipitation Module (TC-PRISMA).

Calculations and simulations for higher-order systems might not be valid beyond the Al-rich region.

Combining Databases

It is possible to combine several databases to make calculations using Thermo-Calc. For more information related to a specific type of problem, contact one of our support specialists at info@thermocalc.com. The experts are available to make recommendations on the most suitable database to use for your needs.

TCS Al-based Alloy Database (TCAL) Resources

Information about the database is available on our website and in the Thermo-Calc software online help.

- **Website**: On our website the information is both searchable and the database specific PDFs are available to download.
- **Online Help**: Technical database information is included with the Thermo-Calc software online help. When in Thermo-Calc, press F1 to search for the same information as is contained in the PDF documents described. Depending on the database, there are additional examples available on the website.

Database Specific Documentation

- The *TCAL: TCS Al-based Alloy Database Technical Information* PDF document contains version specific information such as the binary, ternary and higher-order assessed systems, phases and models. It also includes details about the properties data (e.g. viscosity, surface tension, etc.), a list of the included elements, and summaries of the database revision history by version.
- The *TCAL: TCS Al-based Alloy Database Examples Collection* PDF document contains a series of validation examples using experimental data, and a set of calculation examples showing some of the ways the database can be used.
- Aluminium-based alloys on the Thermo-Calc website also has a variety of information related to the use of this database.

TCAL7 Elements, Systems, Phases and Properties

Included Elements

There are 39 elements included in the most recent version of the database.

Al	Ag	B	Be	Bi	C	Ca	Cd	Ce	Co
Cr	Cu	Er	Fe	Ga	Ge	H	Hf	In	K
La	Li	Mg	Mn	Mo	Na	Nb	Ni	P	Pb
Sc	Si	Sn	Sr	Ti	V	Y	Zn	Zr	

Assessed Systems and Phases

The most recent version of the database contains:

- 267 assessed binary systems, which can be calculated with the BINARY module in Thermo-Calc Console Mode.
- 98 assessed ternary systems, mostly to their full range of composition. These can be calculated with the TERNARY module in Thermo-Calc Console Mode.
- Some quaternaries are assessed within the Al-rich region.
- More than 600 solution and intermetallic phases. This includes nearly all stable phases in the assessed systems and the most important metastable phases that may form in as-cast and aged Al-based alloys. The GAS phase is rejected by default and has to be manually restored if required for a calculation.

In Console Mode, you can list phases and constituents in the Database (TDB) module and the Gibbs (GES) module. For some phases, supplementary information is included in the definitions. To show the information, it is recommended in the Database (TDB) module to use the command LIST_SYSTEM with the option `Constituents`.

Properties Data

A variety of properties data are included with the TCS Al-based Alloy Database (TCAL).

- Electrical Resistivity and Thermal Conductivity Models

- Surface Tension of Metallic Liquid Alloys Model
- Viscosity of the Metallic Liquids Model
- Molar Volume Model

Molar volume with thermal expansion coefficients properties data have been available since TCAL2. Electrical resistivity, thermal conductivity, viscosity of metallic liquids and surface tension of metallic liquids properties data are available starting with TCAL7.

Below is a summary of the available parameters and variables for this database when working in Thermo-Calc. There are differences when you are working in Console Mode versus Graphical Mode as well as if you use the TC-Python SDK. More details are described in the relevant sections. This information is also contained in the online help.

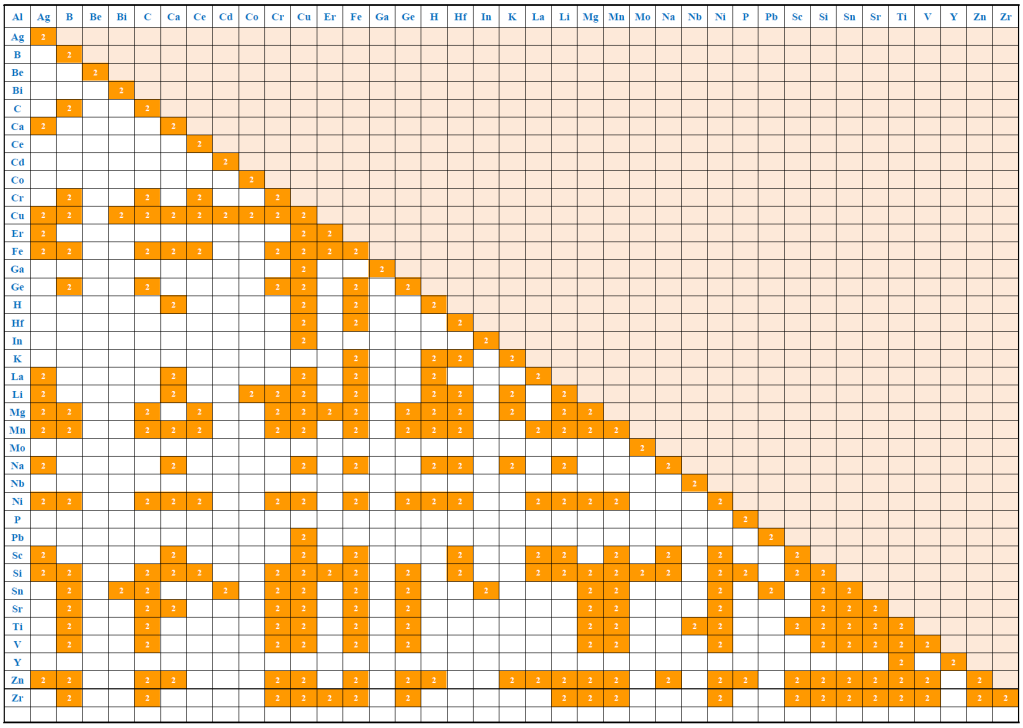
Property	Model Parameters in TDB File	Variables to Show or Plot in Console Mode and TC-Python
Electrical resistivity	ELRS, ESPD	ELRS for a system `ELRS(PHI)` for a phase PHI
Thermal conductivity	THCD	THCD for a system `THCD(PHI)` for phase PHI
Electrical conductivity		ELCD for a system `ELCD(PHI)` for phase PHI
Thermal resistivity		THRS for a system `THRS(PHI)` for phase PHI
Thermal diffusivity		THDF for a system `THDF(PHI)` for phase PHI
Surface tension	SIGM, XI	`SURF(LIQUID)`
Dynamic viscosity	VICS	`DVIS(LIQUID)`
Kinematic viscosity		`KVIS(LIQUID)`
Molar volume	V0, VA	VM for a system `VM(PHI)` for phase PHI

TCAL7 Systems

In this section:

TCAL7 Assessed Binary Systems

These are the assessed binary systems, which are mostly in the full range of composition and temperature.



TCAL7 Assessed Ternary Systems

The assessed ternary systems that are mostly in full compositional ranges.

Ternary Systems
Ag-Al-Cu
Al-Bi-Sn
Al-C-Cr
Al-C-Mg
Al-C-Si
Al-C-V
Al-Cd-Sn
Al-Ce-Cr
Al-Ce-Cu
Al-Ce-Fe
Al-Ce-Mg
Al-Ce-Mn
Al-Ce-Ni
Al-Ce-Si
Al-Cr-Mg
Al-Cr-Si
Al-Cr-Sn
Al-Cu-Er
Al-Cu-Fe

Ternary Systems
Al-Cu-Li
Al-Cu-Mg
Al-Cu-Mn
Al-Cu-Ni
Al-Cu-Sc
Al-Cu-Si
Al-Cu-Sn
Al-Cu-Zn
Al-Er-Fe
Al-Er-Mg
Al-Fe-Mg
Al-Fe-Mn
Al-Fe-Ni
Al-Fe-Si
Al-Fe-Zn
Al-In-Sn
Al-Li-Mg
Al-Li-Si
Al-Li-Zr

Ternary Systems
Al-Mg-Mn
Al-Mg-Ni
Al-Mg-Si
Al-Mg-Ti
Al-Mg-Zn
Al-Mn-Ni
Al-Mn-Si
Al-Mn-Zn
Al-Mo-Si
Al-Nb-Ti
Al-Ni-Si
Al-Ni-Zn
Al-P-Si
Al-P-Zn
Al-Pb-Sn
Al-Sc-Si
Al-Si-Sn
Al-Si-Sr
Al-Sc-Ti

Ternary Systems
Al-Sc-Zr
Al-Si-Ti
Al-Si-Zn
Al-Sn-Zn
Al-Ti-Y
Cu-Fe-Mg
Cu-Fe-Mn
Cu-Fe-Ni
Cu-Fe-Si
Cu-Fe-Zn
Cu-Li-Mg
Cu-Mg-Mn
Cu-Mg-Ni
Cu-Mg-Si
Cu-Mg-Zn
Cu-Mn-Ni
Cu-Mn-Si
Cu-Mn-Zn
Cu-Ni-Si
Cu-Ni-Zn
Cu-Si-Zn
Fe-Mg-Mn
Fe-Mg-Ni

Ternary Systems
Fe-Mg-Si
Fe-Mg-Zn
Fe-Mn-Ni
Fe-Mn-Si
Fe-Mn-Zn
Fe-Ni-Si
Fe-Ni-Zn
Fe-Si-Zn
Mg-Mn-Ni
Mg-Mn-Si
Mg-Mn-Zn
Mg-Ni-Si
Mg-Ni-Zn
Mg-Si-Zn
Mn-Ni-Si
Mn-Ni-Zn
Mn-Si-Zn
Ni-Si-Zn

TCAL7 Assessed Quaternary Systems

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

TCAL7 Phases

In this section:

Common Phases for Aluminum Alloys

TCAL7 Models for the Included Phases

The following lists common phase names and the corresponding Thermo-Calc database phase names for some key aluminum alloys.

Name in the Database	*Common Name and Description*
AL15SI2M4	A cubic precipitate, which originates from the Al-Mn-Si ternary system, aka τ9, Al15Mn3Si2, Al16Mn4Si3 or Al15Mn4Si2. Mn can be substituted by Fe, as well as Cr and Mo. The phase observed in aluminum alloys is also designated as α.
AL13FE4	An iron aluminide, which often forms as a primary phase during casting, aka Al3Fe.
AL2CU_C16	The so-called θ-Al2Cu phase that forms in many Cu-containing aluminum alloys.
AL2CU_OMEGA	Ω-Al2Cu, a metastable precipitate and the coherent version of the θ phase
THETA_PRIME	A semi-coherent precipitate with a stoichiometry of Al2Cu in α-(Al), i.e. the GPI zones.
THETA_DPRIME	Coherent metastable precipitates in α-(Al), also referred to as GPII zones. It has a stoichiometry close to Al3Cu.
BETA_DPRIME	Metastable precipitate β'' related to Mg2Si that forms in Al-Mg-Si based alloys. It may contain Al atoms (Al2Mg5Si4) or be Al-free (Mg5Si6).
BETA_PRIME	Metastable precipitate β' related to Mg2Si, aka Mg9Si5/Mg1.8Si
U1_AL2MGSI2	An Al-containing pre-β Al-Mg-Si metastable precipitate, U1_Al2MgSi2
U2_AL4MG4SI4	An Al-containing pre-β Al-Mg-Si metastable precipitate, U2_Al4Mg4Si4
AL18FE2MG7SI10	A quaternary phase, aka Al8FeMg3Si6, Q, PHI and H_PHASE
AL6MN	A common Al-Mn compound that forms in Mn-containing aluminum alloys. Mn could be substituted by Cu and Fe, especially to a larger extent by the latter.
AL28CU4MN7	An Al-Cu-Mn intermetallic phase that forms in aluminum alloys
Q_ALCUMGSI	A stable Al-Cu-Mg-Si quaternary phase, aka Q, Al5Cu2Mg8Si6, Al3Cu2Mg9Si7 and Al4Cu2Mg8Si7
QPRIME	The coherent / semi-coherent version of Q_ALCUMGSI
MG2SI_C1	Mg2Si, which forms in Mg- and Si-containing aluminum alloys

Name in the Database	*Common Name and Description*
AL9FE2SI2	A common Al-Fe-Si ternary phase in aluminum alloys, aka τ6, Al5FeSi, β-AlFeSi
AL8FE2SI	A common Al-Fe-Si ternary phase in aluminum alloys, aka τ5, α-AlFeSi
AL7CU2FE	An Al-Cu-Fe ternary compound that may form in some aluminum alloys
DIAMOND_A4	Si, as well as C and Ge
C14_LAVES	A common stable precipitate in 7000 series aluminum alloys, aka. the η (MgZn2) phase, eta and the M phase. This phase includes all MgZn2-type phases.
ETA_PRIME	The metastable η' phase, which is related to the η-MgZn2 phase.
T_PHASE	A stable phase in Al-Mg-Zn, Al-Cu-Mg and Al-Cu-Mg-Zn. It is modeled as (Al,Cu,Zn)49Mg32 and is often designated as Al2Mg3Zn3 in aluminum alloys.
T_PRIME	The metastable form of T phase, T’
S_PHASE	The S phase, Al2CuMg
S_PRIME	The metastable S’ phase, precursor to the S phase
Q_ALCUMGSI	The Al-Cu-Mg-Si quaternary phase, i.e. the Q Phase, aka Al5Cu2Mg8Si6, Al3Cu2Mg9Si7 and Al4Cu2Mg8Si7
Q_AL7CU3MG6	An Al-Cu-Mg ternary phase, aka, Al7Cu3Mg6 and the Q phase

TCAL7 Models for the Included Phases

Phase Models
AG2CA (Ag)0.666667(Ca)0.333333
AG2ER (Ag)2(Er)1
AG2LA (La)1(Ag)2
AG2NA (Ag)2(Na)1
AG4SC (Ag)0.8(Sc)0.2
AG51ER14 (Ag)0.77(Er)0.23
AG51LA14 (La)14(Ag)51
AG5LA (La)1(Ag)5
AG5ZN8 (Zn,Ag)2(Ag)2(Ag,Zn)3(Zn,Ag)6
AG7CA2 (Ag)0.777778(Ca)0.222222
AG9CA2 (Ag)0.818182(Ca)0.181818
AGCA3 (Ag)0.25(Ca)0.75
AGER

Phase Models
(Ag)1(Er)1
AGLA (La)1(Ag)1
AGMG3: > Ag17Mg54 (Ag)0.23(Mg)0.77
AGMG4: > Ag9Mg37 (Ag)0.2(Mg)0.8
AGSC (Ag)0.5(Sc)0.5
AGZN3 (Zn,Ag)1
AGZN_HP9 (Zn)1(Ag,Zn)2
AL10CE2M7: > T2 (Cr,Al,Mn,Cu,Fe)0.8947(Er,Ce)0.1053
AL10CEFE2 (Al)10(Ce,Er)1(Fe)2
AL10CU10FE (Fe)1(Cu,Al)10(Al)10
AL10FE3NI (Al)5(Ni,Fe)2
AL11CE3 (Al,Mg)0.7857(Ce)0.2143
AL11CU5MN3 (Al)11(Mn)3(Cu)5
AL11LA3_HT

Phase Models
(Al)11(La)3
AL11LA3_LT (Al)11(La)3
AL11MN3ZN2 (Mn)3(Zn)2(Al)11
AL11MN4_HT (Mn,Al)29(Mn)10
AL11MN4_LT (Al,Zn)11(Fe,Mn)4
AL12MN (Al)12(Mn)1
AL12MO (Si,Al)12(Mo)1
AL13CEMG6 (Al)0.667(Ce)0.05(Mg)0.283
AL13CO4 (Al)13(Co)4
AL13CR4SI4: > Al-Cr-Si, tao 1 (Al)13(Cr)4(Si)4
AL13FE4: > solution phases based on Al13Fe4, aka Al3Fe (Al,Cu)0.6275(Zn,Mn,Ni,Fe)0.235(Si,Al,Zn,Va)0.1375
AL13NI38ZN49: > Al-Ni-Zn ternary phase (Al)0.13(Ni)0.38(Zn)0.49
AL14CA13 (Mg,Al,Zn)14(Ca)13
AL15SI2M4: > Solution of Al-Mn-Si ternary phase, tao 9, Al15(Mn,Fe)3Si2

Phase Models
(Al)16(Mo,Mn,Fe,Cr)4(Si)1(Al,Si)2
AL17MO4 (Si,Al)17(Mo)4
AL18FE2MG7SI10: > Quaternary phase, aka Al8FeMg3Si6 and Q_/PHI/H_PHASE (Al)18(Fe)2(Mg)7(Si)10
AL18MG3TM2 (Al,Mg)18(Al,Mg)3(Ti,Cr,Mn)2
AL1CE1SI1: > tI12, I4_1md (Si,Al)2(Ce)1
AL1CE2 (Al)0.3333(Ce)0.6667
AL1LI2 (Al)1(Li)2
AL1MN1SI1: > the Al-Mn-Si ternary phase, tao3 (Al)1(Mn)1(Si)1
AL20CECR2 (Al)0.869565(Ce)0.043478(Cr)0.086957
AL21V2 (Al)21(V)2
AL22MO5 (Si,Al)22(Mo)5
AL23CE4NI6: > T8 (Al)23(Ce)4(Ni)6
AL23V4 (Al)23(V)4
AL24MN5ZN

Phase Models
(Zn,Mn)5(Zn)1(Al)24
AL28CU4MN7 (Al)28(Mn)7(Cu)4
AL2CENI: > T2 (Al)2(Ce)1(Ni)1
AL2CULI: > Al-Cu-Li ternary phase, i.e. T1 (Al)0.5(Cu)0.25(Li)0.25
AL2CU_C16: > Al2Cu,AlHf2,Fe2B,FeGe2,FeZr2,FeSn2,Mn2B,MnSn2,NiB2,NiZr2,SiZr2 (Al,Hf,Ni,Fe,Zr,Mn,Sn,Ge)2(Fe,Ni,Cu,Mn,B,Al,Si)1
AL2CU_OMEGA: > Al2Cu-OMEGA metastable precipitate (Al)2(Cu)1
AL2ER3 (Al,Mg)0.4(Er)0.6
AL2FE1 (Si,Cu,Al,Zn)2(Mn,Ni,Fe)1
AL2LI3 (Mg,Al)2(Li)3
AL2MGC2 (Al)2(Mg)1(C)2
AL2MN2SI3: > the Al-Mn-Si ternary phase, tao1 (Al)2(Mn)2(Si)3
AL2MNSI3: > the Al-Mn-Si ternary phase, tao10 (Al)2(Mn)1(Si)3
AL2SC (Sc,Zr,Ti)1(Al)2
AL2SI2SR

Phase Models
(Al)2(Si)2(Sr)1
AL2SR_OI12: > Al2Sr, SrZn2 (Zn,Al)2(Sr)1
AL2TI (Ti,Nb,Al)2(Ti,Nb,Sc,Al)1
AL2Y_C15 (Y,Al)2(Y,Al)1
AL2ZR3_TP20: > Al2Zr3, Al2Hf3, ZN2Zr3 (Al,Zn)2(Zr,Sc,Y,Hf)3
AL31MN6NI2: > Orthorhombic, ternary Al-Mn-Ni phase (Al)31(Mn)6(Ni)2
AL3CA8 (Al)3(Mg,Ca)8
AL3CECU: > T3 (Cu,Al)0.8(Ce)0.2
AL3CE_H (Al)0.75(Ce)0.25
AL3CE_L (Si,Al)0.75(Ce)0.25
AL3CO (Al)3(Co)1
AL3CU1ER1 (Al)0.6(Cu)0.2(Er)0.2
AL3HF4 (Al)3(Hf)4
AL3LA

Phase Models
(Al)3(La)1
AL3LI8SI5 (Li)0.5(Al)0.1875(Si)0.3125
AL3MN4SI2: > the Al-Mn-Si ternary phase, tao5 (Al)3(Mn)4(Si)2
AL3MNSI2: > the Al-Mn-Si ternary phase, tao4 (Al)3(Mn)1(Si)2
AL3MO (Si,Al)3(Mo)1
AL3NI2 (Si,Al,Zn)3(Al,Fe,Mg,Cu,Ni)2(Ni,Va)1
AL3NI5 (Al)0.375(Ni)0.625
AL3NI_D011 (Ni,Mn,Al)0.75(Ni,B,C,Fe)0.25
AL3TI_D022: > Al3Ti, Ni3V, GeMn3, Al3V (Nb,Mn,Ni,Si,Al,Ti)3(Ge,Nb,Zr,Ti,Sc,Mn,V,Al)1
AL3TI_LT (Si,Nb,Ti,Al)3(Ti,Al,Nb,Sc)1
AL3X: > Al3Sc (dissolving Ti, Zr), Al3Li (Zr,Er,Sc,Li,Ti)1(Al,Si,Mg)3
AL3Y_HT (Al)0.75(Y)0.25
AL3Y_LT (Al)0.75(Y)0.25
AL3ZR2_OF40: > Al3Zr2, Al3Hf2

Phase Models
(Al,Li)3(Sc,Zr,Hf)2
AL3ZR5_D8M: > Al3Zr5, Cr3Si5, Ge3V5, Si3V5 (Ge,Al,Si)3(Cr,Zr,V)5
AL3ZR_D023: > Al3Zr, Al3Hf (Li,Al)3(Zr,Hf,Sc,Ti)1
AL40CE30NI30: > T12 (Al)0.403(Ce)0.304(Ni)0.293
AL45V7: > Al45Cr7, Al45V7 (Al)45(V,Cr)7
AL4C3 (Si,Al)2(Mg,Si,Al)2(C)3
AL4C4SI (Al)4(Si)1(C)4
AL4CE1 (Al)0.8(Ce)0.2
AL4CE3SI6 (Al)4(Ce)3(Si)6
AL4CENI: > T5 (Al)4(Ce)1(Ni)1
AL4CR (Cr)1(Va,Al,Si)4
AL4FE (Al)4.2(Fe)1
AL4LI9 (Al)4(Li)9
AL4MN_R: > AL461MN107

Phase Models
(Al)0.81162(Mn,Fe)0.18838
AL4MN_U (Zn,Al)4(Mn)1
AL4MO (Al,Si)4(Mo)1
AL4M_D13: > Al4Ca, Al4Sr (Si,Al)4(Sr,Ca)1
AL4ZR5 (Al)4(Sc,Zr)5
AL53LA22 (Al)0.707(La)0.293
AL5CE1NI2: > T6 (Al)5(Ce)1(Ni)2
AL5CE2NI5: > T3, 13 (Al)0.35(Ce)0.165(Ni)0.485
AL5CO2 (Al)5(Co)2
AL5CR (Si,Al)5(Cr)1
AL5CU3ER2 (Al)0.5(Cu)0.3(Er)0.2
AL5FE2 (Zn,Cu,Si,Al)5(Ni,Fe,Mn)2
AL5FE4 (Fe,Cu,Mn,Al)1
AL5MN6SI7: > the Al-Mn-Si ternary phase, tao2

Phase Models
(Al)5(Mn)6(Si)7
AL5MO (Si,Al)5(Mo)1
AL5TI2 (Ti,Nb,Al)5(Ti,Al,Nb)2
AL5TI3 (Al)5(Nb,Ti)3
AL60CE12NI28: > T11 (Al)0.6(Ce)0.12(Ni)0.28
AL62CU25FE13 (Fe)0.125(Cu,Al)0.255(Al)0.62
AL63MO37 (Si,Al)0.63(Mo)0.37
AL6ER2FE11 (Al)6(Er)2(Fe)11
AL6MN (Al,Cu,Zn)6(Mn,Cu,Fe)1
AL6NI3SI (Al)6(Ni)3(Si)1
AL71FE5NI24 (Al)0.71(Fe)0.05(Ni)0.24
AL7CE5SI3 (Al)0.49(Ce)0.333333(Si)0.176667
AL7CU2FE: > Solution phase of the ternary compound Al7Cu2Fe (Fe,Ni)1(Cu)2(Al)7
AL7CU4NI

Phase Models
(Al)1(Va,Ni,Cu,Fe)1
AL7ERMG2 (Al)0.66667(Er)0.1(Mg)0.23333
AL7SR8 (Al)7(Sr)8
AL8C7SI (Al)8(Si)1(C)7
AL8CEFE2 (Al)8(Ce)1(Fe)2
AL8CEM4: > T1 (Al)0.6154(Er,Ce)0.0769(Fe,Cu,Cr,Mn,Al)0.3077
AL8FE2SI: > solution of the Al-Fe-Si ternary phase, tao 5, alpha_AlFeSi (Al)0.6612(Fe,Mn)0.19(Si)0.0496(Al,Si)0.0992
AL8MN5 (Zn,Al)12(Mn)5(Mn,Si,Cu,Al)9
AL8MO3 (Al,Si)8(Mo)3
AL8V5 (Al,V)2(V)2(Al,V)3(Al)6
AL9CO2 (Al)9(Co)2
AL9CR3SI: > Al-Cr-Si, tao 2 (Al)9(Cr)3(Si)1
AL9CU6ER5 (Al)0.45(Cu)0.3(Er)0.25
AL9FE2SI2: > Al-Fe-Si ternary phase, tao 6, aka Al5FeSi, beta_AlFeSi

Phase Models
(Al)0.598(Mn,Fe)0.152(Si)0.1(Si,Al)0.15
AL9FENI (Al)9(Fe,Ni)2
AL9MN2ZN (Mn)2(Zn)1(Al)9
ALB12 (Al)1(B)12
ALB2_C32: > AlB2, B2Cr, B2Mg, B2Mn, B2Ti, B2V, B2Zr (Al,Mg,Zr,Ti,Mn,V,Cr)1(B)2
ALC3V4 (V)4(Al)1(C)2(Va,C)1
ALCCR2: > Prototype AlCCr2 (hP8) (Al)1(C)1(V,Cr)2
ALCE2CU2: > T5 (Al)0.2(Ce)0.4(Cu)0.4
ALCE3_H (Al)0.25(Ce)0.75
ALCE3_L (Al)0.25(Ce)0.75
ALCEFE (Fe,Al)2(Ce)1
ALCEM: > T4 (Al)0.3333(Ce,Er)0.3333(Ni,Cu)0.3334
ALCESI2 (Al)1(Ce)1(Si)2
ALCE_OC16

Phase Models
(Al)0.5(Ce)0.5
ALCRSI_T3: > Al-Cr-Si, tao 3 (Al,Si)11(Cr)4
ALCRSI_T4: > Al-Cr-Si, tao 4, AL58CR32SI11 (Al)58(Cr)31.5(Si)10.5
ALCR_GAMMA1 (Si,Al,Cr)2(Cr)2(Al,Cr)3(Al,Si)6
ALCU3MN2 (Al)1(Mn)2(Cu)3
ALCULI_B: > Al-Cu-Li ternary phase, TB (Al)0.6(Cu)0.32(Li)0.08
ALCULI_R: > Al-Cu-Li ternary phase, R (Al)0.55(Cu)0.117(Li)0.333
ALCULI_T2: > Al-Cu-Li ternary phase, T2 (Al)0.57(Cu)0.11(Li)0.32
ALCUSC_TAU (Cu,Al)0.6154(Al,Cu)0.3077(Sc)0.0769
ALCU_DEL (Zn,Al)2(Fe,Cu)3
ALCU_EPS (Ni,Cu,Zn,Al)1(Cu,Fe)1
ALCU_ETA (Al,Cu)1(Zn,Ni,Cu,Fe)1
ALCU_ZETA (Al)9(Cu,Fe)11
ALER2

Phase Models
(Mg,Al)0.33333(Er)0.66667
ALER_OP16 (Mg,Al)0.5(Er)0.5
ALFESI_T10: > Al-Fe-Si ternary phase, AL60FE25SI15, tao 10 (Al)0.6(Fe)0.25(Si)0.15
ALFESI_T11: > Al-Fe-Si ternary phase, AL85FE30SI15, tao 11 (Al)0.65(Fe)0.25(Si)0.1
ALFESI_T2: > Al-Fe-Si ternary phase, tao 2, gamma_AlFeSi (Al)0.5(Fe)0.2(Si)0.1(Al,Si)0.2
ALFESI_T3: > Al-Fe-Si ternary phase, AL56FE24SI10, tao 3 (Al)0.56(Fe)0.24(Si)0.2
ALFESI_T4: > Al-Fe-Si ternary phase, tao 4, delta_AlFeSi (Al)0.4166(Fe)0.1667(Si)0.25(Al,Si)0.1667
ALFESI_T7: > Al-Fe-Si ternary phase, AL9FE5SI6, tao 7 (Si,Al)3(Fe)1
ALFESI_T8: > Al-Fe-Si ternary phase, AL2FE3SI4, tao 8 (Al,Si)2(Fe)1
ALFESI_T9: > Al-Fe-Si ternary phase, tao 1 / tao 9 (Al,Si)5(Fe)3
ALFEZN_GAMMA: > Al-Fe-Zn ternary phase, aka gamma 2, no detailed structure (Fe,Zn,Al)0.255(Zn)0.745
ALLA (Al)1(La)1
ALLI2ZR (Al)1(Li)2(Zr)1
ALLI5SI2

Phase Models
(Li)0.6625(Al)0.0875(Si)0.25
ALLIMG_T (Al)0.53(Li)0.33(Mg)0.14
ALLISI (Li)0.333333(Al)0.333333(Si)0.333334
ALM3_A15: > A15 (Si,Mo,Nb,Al,Ti)1(Nb,Mo,Ti,Al)3
ALMG3NI2: > Ternary phase AlMg3Ni2, cF96, Fd-3m, Ti2Ni type (Al)1(Ni)2(Mg)3
ALMGZN_PHI: > a Al-Mg-Zn ternary phase know as PHI (Mg)6(Al,Zn)5
ALMG_BETA (Li,Mg)89(Al,Zn)140
ALMG_EPS (Mg)23(Zn,Al)30
ALMG_GAMMA (Mg,Li)5(Zn,Al,Mg)12(Al,Zn,Mg)12
ALMNSI_T6: > the Al-Mn-Si ternary phase, tao6 (Al,Mn)4(Si)1
ALMNSI_T8: > the Al-Mn-Si ternary phase, tao 8 (Al)6(Mn)3(Mn,Al,Si)3(Si,Al)1
ALNB2 (Ti,Nb,Al)10(Ti,Nb)4(Al,Nb,Ti)16
ALNI16SI9 (Al)1(Ni)16(Si)9
ALNI2SI

Phase Models
(Va,Al,Si)1(Ni)1
ALNI2ZN (Al)0.25(Ni)0.5(Zn)0.25
ALP (Al)1(P)1
ALSC2SI2 (Al)1(Sc)2(Si)2
ALSC_OP (Zr,Sc)1(Al)1
ALSI3TI2: > Al-Si-Ti Tao 2 (Al,Si)0.2(Si)0.466667(Ti)0.333333
ALSI7TI4: > Al-Si-Ti Tao 1 (Al,Si)0.1(Si)0.566667(Ti)0.333333
ALSISR (Al,Si)2(Sr)1
ALTI3_D019 (Al,Ti,Nb)3(Si,Al,Ti,Nb)1
ALY_B33 (Al)1(Y)1
ALZR2_B82: > SnTi2, GeMn2, AlZr2, AlSc2 (Al,Ge,Va,Sn,Mn)1(Mn,Ti,Va,Sc,Y,Zr)2
B2_BCC: > CuZr, FeTi, TiZn, ZnZr, MnZn(rt), AlCo (Cu,Al,Co,Zn,Fe)1(Ti,Va,Zr,Mn,Co)1
B32_ALLI (Mg,Li,Al)1(Li,Va,Mg)1
B4C

Phase Models
(B12,B11C)1(C2B,B2,Cb2)1
B82_OMEGA (Al)1(Ti,Nb)1(Ti)1
BCC_A2: > Metallic BCC_A2 solution (Zr,Mg,Sn,Nb,Ga,Ag,In,Ge,V,Mn,Ce,La,Li,Y,Al,Sr,P,Zn,Cr,Ni,Cu,Co,Ca,Pb,Mo,Hf,Si,Ti,Sc,Er,Be,Bi,Na,K,Fe,Cd,Va)1(C,Va,B,H)3
BCC_B2: > Solution of ordered BCC_B2, having Gibbs energy contribution from BCC_A2 (Bi,Co,Mg,La,Sc,Ga,Pb,K,Cu,Cd,Li,Fe,Sr,Ni,Ce,Zn,In,Ag,Zr,Mo,Er,Ti,Hf,Cr,Be,Si,Al,Nb,Mn,Va,Ca,Na,Sn,Ge,V)0.5 (Sc,Zn,Va,Mn,V,Ti,Ga,Al,Zr,Mg,Cr,Co,Sn,Hf,Bi,Sr,Si,In,Cu,Ca,Mo,Pb,Ge,Nb,Fe,Ni,Li,Ag,Na,Ce,Cd,Be,La,Er,K)0.5(Va,B,H,C)3
BCC_B32 (Li,Zn)1(Zn,Li)1
BCT_A5: > Pure Sn or its solution (Ti,Sn,Bi,Cd,B,Zn,Pb,Ga,Cu,Al,Ge,In)1
BETA_DPRIME: > metastable beta double prime, related to Mg2Si, Mg5Si6, Al2Mg5Si4 (Si,Al)2(Mg)5(Si)4
BETA_PRIME: > metastable precipitate, Mg9Si5/Mg1.8Si, related to Mg2Si (Mg)1.8(Si)1
BETA_RHOMBO_B (B)93(Si,C,Cu,B)12
B_PRIME: > metastable precipitate, B_Prime, Al-containing Pre-beta phase (Al)3(Mg)9(Si)7
C14_FE2HF (Fe)0.6667(Hf,Fe)0.3333
C14_LAVES: > Solution of MgZn2-type phases, including MgZn2 (Eta, aka M or sigma) (Mn,Al,Mg,Cr,Zn,Ti,Cu,Ni,Li,Fe,Hf,Zr)2(Mn,Hf,Cu,Al,Zr,Er,Fe,Cr,Mg,Sc,Ti,Zn)1
C15_FE2HF (Fe)0.6667(Hf)0.3333

Phase Models
C15_LAVES: > Solution of Cu2Mg-type phases, cF24, Fd-3m (Li,Hf,Si,Ca,Sc,Fe,Cu,Cr,Zr,Mg,La,Al,Ni,Ti,Zn)2(Fe,Sc,Cr,Ce,Si,Cu,Ca,Li,Al,Zr,Ni,Mg,La,Ti,Hf,Er,Zn)1
C36_FE2HF (Fe)0.6667(Hf)0.3333
C36_LAVES: > Solution of MgNi2-type phases, hP24, P63/mmc (Zn,Hf,Fe,Mn,Mg,Zr,Ni,Cu,Cr,Al)2(Cu,Ni,Mg,Al,Fe,Cr,Sc,Hf,Zr,Zn)1
C40_MOSI2 (Si,Al)2(Mo)1
C54_MOSI2 (Si,Al)2(Mo)1
CA14SI19 (Ca)0.424242(Si)0.575758
CA1CU1 (Ca)1(Cu)1
CA2CU (Ca)2(Cu)1
CA2NI7 (Ca)2(Ni)7
CA3SI4 (Ca)0.428571(Si)0.571429
CA3ZN (Ca)3(Zn)1
CA5ZN3 (Ca)5(Zn)3
CACU5_D2D: > CaCu5, CaNi5, CaZn5, Cu5Sr, ScNi5, SrZn5 (Ca,Sc,Sr)1(Ni,Zn,Cu)5

Phase Models
CAH2_HT (Ca)1(H)2
CAH2_LT (Ca)1(H)2
CALI2 (Li)2(Ca)1
CANI3 (Ca)0.25(Ni)0.75
CASI2 (Ca)0.333333(Si)0.666667
CAZN11 (Ca)1(Zn)11
CAZN13_CF112: > CaZn13, SrZn13 (Ca,Sr)1(Zn)13
CAZN2 (Ca)1(Zn)2
CAZN3 (Ca)1(Zn)3
CAZN_OC8 (Ca)1(Zn)1
CBCC_A12 (Sr,Li,V,Sn,Ge,Fe,Mn,Cr,Co,Al,Si,Ni,Ti,Zn,Cu,Zr,Mg)1(H,C,Va,B)1
CD10CU3 (Cd)0.7692(Cu)0.2308
CD3CU4 (Cd)0.4286(Cu)0.5714

Phase Models
CD8CU5 (Cu)2(Cu,Cd)3(Cu)2(Cd,Cu)6
CDCU2 (Cd)1(Cu)2
CE2FE17 (Ce)2(Fe,Al)17
CE2NI7 (Ce)0.222222(Ni,Al)0.777778
CE3SI2 (Ce)3(Si)2
CE3SI4 (Ce)1(Si)1.34
CE3SI5 (Ce)0.37(Si)0.63
CE5SI3 (Si)3(Ce)5
CE5SI4 (Ce)5(Si)4
CE7NI3 (Ce)0.7(Ni)0.3
CENI2 (Ni,Ce)0.333333(Ni,Ce)0.666667
CENI3 (Ce)0.25(Ni,Al)0.75
CENI5 (Ni,Ce,Er)0.166667(Al,Ce,Ni,Cu)0.833333

Phase Models
CENI_OC8 (Ce)0.5(Ni)0.5
CESI2 (Ce)1(Si,Al)2
CESI_OP8 (Ce)1(Si)1
CO2SI_C23: > Ca2Si, Ni2Si, SiSr2, SnSr2, GeSr2 (Cu,Ni,Ca,Sr,Fe)2(Al,Zn,Ge,Si,Sn)1
CR11GE19 (Cr)0.367(Ge)0.633
CR2B_ORTH (Cr)0.666667(B)0.333333
CR3C2 (Cr)3(C)2
CR3GE (Ge,Cr)0.75(Ge,Cr)0.25
CR3MN5 (Cr)3(Mn)5
CR3SI_A15 (Si,Cr)3(Si,Cr,Al)1
CR5B3_D81: > Ca5Si3, Sn3Sr5, Si4Sr5, Ge3Sr5, B3Cr5 (Sr,Cr,Ca)0.625(Si,Ge,B,Ag,Sn)0.375
CR5GE3_HT (Cr,Ge)0.625(Ge,Cr)0.375
CR5GE3_LT (Ge,Cr)0.625(Ge,Cr)0.375

Phase Models
CRB4 (Cr)0.2(B)0.8
CRB_B33: > AgCa, AlHf, AlZr, BNi, BV, GeSr, NiZr, SiSr, SnSr (Ca,Ni,V,Sr,Cr,Al)1(Ge,Zr,Sc,Si,B,Sn,Ag,Hf)1
CRSI2_C40 (V,Si,Cr)1(Cr,Al,Si)2
CRZN13 (Cr)1(Zn)13
CRZN17 (Cr)1(Zn)17
CU10HF7 (Cu)10(Hf)7
CU10SN3 (Cu,Sn)1
CU10ZR7 (Cu)10(Zr)7
CU11IN9 (Cu)0.55(In)0.45
CU15SI4_EPSILON (Mn,Cu,Zn,Mg)0.789474(Si,Al)0.210526
CU16MG6SI7 (Cu)16(Mg)6(Si)7
CU1HF2 (Cu)1(Hf)2
CU1LA1 (Cu)1(La)1

Phase Models
CU2CE (Cu)2(Ce)1
CU2ER (Cu,Al)2(Er)1
CU2IN_HT (Cu)0.545(In,Cu)0.122(In)0.333
CU2IN_LT (Cu)0.64(In)0.36
CU2LA1 (Cu)2(La)1
CU2SC_C11B (Ag,Cu)2(Sc)1
CU2TI (Cu)2(Ti)1
CU33SI7_DELTA (Cu,Zn)0.825(Si)0.175
CU37LA3 (Cu)37(La)3
CU3MG2SI (Cu)2.74(Mg)2(Si)1.26
CU3SN (Sn,Cu)3(Sn,Cu)1
CU3TI2 (Cu)3(Ti)2
CU41SN11 (Cu,Sn)41(Sn,Cu)11

Phase Models
CU46NI25SI29 (Cu)0.458(Ni)0.25(Si)0.292
CU4CE (Cu,Al)4(Ce)1
CU4LA1 (Cu)4(La)1
CU4SC (Cu)4(Sc)1
CU4TI1 (Cu,Ti)4(Cu,Ti)1
CU4TI3 (Cu)4(Ti)3
CU51HF14 (Cu)51(Hf)14
CU51ZR14 (Cu)51(Zr)14
CU56SI11_GAMMA (Mn,Zn,Cu,Si,Ni,Mg)0.835821(Si)0.164179
CU5CE (Al,Cu)5(Ce)1
CU5ER_C15B (Cu)5(Er)1
CU5HF (Cu)5(Hf)1
CU5LA1 (Cu)5(La)1

Phase Models
CU5MN4SI (Cu)0.5(Mn)0.37(Si)0.13
CU6CE (Cu)6(Ce)1
CU6LA1_HT (Cu)6(La)1
CU6LA1_LT (Cu)6(La)1
CU6NISI3 (Ni,Cu)0.732(Si)0.268
CU6SN5_HT (Cu)1(Sn,Cu)1(Sn)1
CU6SN5_LT (Cu)1(Sn,Cu)1(Sn)1
CU7ER2 (Cu)7(Er)2
CU8HF3 (Cu)8(Hf)3
CU8ZR3 (Cu)8(Zr)3
CU9ER2 (Cu)9(Er)2
CU9GA4_0 (Cu)6(Ga,Cu)6(Ga)1
CU9GA4_1 (Cu)6(Ga,Cu)3(Ga,Cu)3(Ga)1

Phase Models
CU9GA4_2 (Cu)3(Va,Cu)3(Ga,Cu)3(Ga)4
CU9GA4_3 (Va,Cu)6(Ga,Cu)3(Ga)4
CUB_A13 (Ag,Ti,Mn,Zr,Ni,Mg,Cu,V,Ge,Ce,Sn,Hf,Sr,Si,Li,Cr,Al,Zn,Fe)1(Va,H,B,C)1
CUCE (Cu)1(Ce)1
CUER_B2 (Cu,Al)1(Er)1
CUGA2 (Cu)1(Ga)2
CUGA_THETA (Cu)0.778(Ga)0.222
CUIN_GAMMA (Cu)2(Cu,In)2(Cu)3(Cu,In)6
CUIN_THETE (Cu)0.7(In)0.3
CULIMG_T (Cu)1(Li)0.08(Mg)1.92
CUMG2 (Ni,Cu)1(Mg)2
CUMNZN (Cu)0.334(Mn)0.333(Zn)0.333
CUSC (Cu)1(Sc)1

Phase Models
CUSI_ETA (Ni,Cu,Zn,Mn)0.76(Si)0.24
CUSN_GAMMA (Sn,Cu)1
CUSR (Sr)1(Cu)1
CUTI3 (Ti,Cu)1(Ti)3
CUTI_B11 (Ti,Cu)1(Ti,Cu)1
CUZR2_C11B: > AlCr2, CuTi2, CuZr2, Ti2Zn, ZnZr2 (Al,Zn,Cr,Si,Cu)1(Ti,Cr,Al,Zr)2
DHCP (La,Sc,Cu,Ce,Ni)1
DIAMOND_A4: > Pure C, Ge, Si or solution phases based on them (Ti,Zn,Ga,Al,Si,P,B,Sr,C,Sn,Ge)1
EPSILON (Mn,Cu,Zn)1
ER5SI3 (Er)0.625(Si)0.375
ER5SI4 (Er)0.555556(Si)0.444444
ERSI2 (Er)0.37(Si)0.63
ERSI_OC8 (Er)0.51(Si)0.49

Phase Models
ERSI_OP8 (Er)0.5(Si)0.5
ETA_PRIME: > metastable precipitate, related to MgZn2-based Eta phase (Al)0.21(Mg)0.28(Zn,Cu)0.51
FCC_A1: > Metallic FCC_A1 solution, e.g. (Al), (Cu), and MC carbides (Nb,Ga,Sc,Be,Er,Co,Fe,P,Sr,Cd,Pb,Al,Ag,Ni,Bi,In,Na,Ge,Si,La,Zn,Li,Ca,Mg,Mo,Cu,Zr,Ce,Hf,Cr,Ti,Mn,K,Sn,V)1(H,B,Va,C)1
FE17ER2 (Al,Fe)17(Er)2
FE1HF2 (Fe)0.3333(Hf)0.6667
FE23ER6 (Al,Fe)23(Er)6
FE2GE1 (Fe)1(Fe,Va)1(Ge)1
FE2GE3 (Fe)2(Ge)3
FE2SC_C15 (Fe)0.64(Sc)0.36
FE2SI (Ni,Fe)2(Si,Al)1
FE3ER (Fe)3(Er)1
FE3SN2 (Fe)3(Sn)2
FE5NI3SI2 (Ni,Fe)4(Si)1

Phase Models
FE5SN3_D82 (Fe)5(Sn)3
FE6GE5 (Fe)6(Ge)5
FE6SC29 (Fe)0.17(Sc)0.83
FEB_B27: > BFe, BMn, BTi, GeZr, SiTi, SrZn, SiZr (Ti,Zr,Sr,Fe,Mn)1(Si,Zn,Ge,B)1
FEGE_ETA (Fe)13(Ge)9
FEM_B35: > FeSn, FeGe (Fe)1(Ge,Sn)1
FESI2_H (Fe,Ni)3(Si,Al,Mg)7
FESI2_L (Ni,Fe)1(Al,Si)2
FESI_B20: > FeSi, MnSi, CrSi, CrGe (Mn,Fe,Ni,Cr)1(Si,Al,Mg,Ge)1
FEZN_DELTA (Fe)0.058(Si,Ni,Zn,Fe,Al,Mn,Cu)0.18(Zn)0.525(Zn)0.237
FEZN_GAMMA1 (Fe)0.137(Fe,Zn,Si,Cu,Al,Ni)0.118(Zn,Mn)0.745
FEZN_ZETA (Ni,Fe,Va,Mn)0.072(Al,Zn)0.856(Si,Al,Cu,Zn,Va)0.072
FEZR3 (Fe)1(Zr)3

Phase Models
GAMMA_D810 (Al,Si)12(Cr)5(Si,Al,Cr)9
GAMMA_D82 (Zn,Fe,Mn)2(Ni,Mn,Zn,Fe)2(Zn,Fe,Si,Al,Mn,Cu,Ni)3(Al,Zn)6
GAMMA_D83: > solution between Al8Cu5 (rt) and Cu5Zn8 (Zn,Al,Fe,Ni,Si)4(Si,Al,Zn,Ni,Cu)1(Fe,Ni,Ag,Mn,Cu,Zn)8
GAMMA_H: > Cu5Zn8-type Al8Cu5 (ht) phase (Al,Zn)4(Cu,Al,Zn)1(Ni,Mn,Cu,Fe)8
GAS (Sr2,Zn,K2,Cu2,C4,Si,C,Fe,Mn,C3,Ge,B,P2,Li,Ca,Al,P,Cu,C2,Al1H1,Si3,H2,Co,Al1C1,Fe2,C60,Ti2,K,Al2,Sn2,Ni2,Ti,Sr,H1Na1,Co2,P4, Na,H1Li1,V,Cu1H1,Al1H3,K1Li1,Al1H2,Li2,Sn,Cr,Ca1H1,Na2,Cr2,Mg2,H,Ca2,B2,Sc,Ni,Si4,C5,Ge2,Mg,Si2)1
GE12NI19 (Ge,Ni)0.613(Ni,Ge)0.387
GE2MN3 (Ge)2(Mn)3
GE2MN5 (Mn,Ge)2(Mn)5
GE2NI3 (Ni,Ge)0.6(Ge)0.4
GE2NI5 (Ni)0.72(Ge)0.28
GE2SR (Ge)2(Sr)1
GE3MN7 (Ge)3(Mn)7
GE3NI5_HT (Ge,Ni)0.625(Ni,Ge)0.375

Phase Models
GE3NI5_LT (Ni)0.63(Ge)0.37
GE3TI5 (Ti)5(Ge)3
GEMN3_HT (Mn,Ge)1(Mn)3
GENI2 (Ni)0.665(Ge)0.335
GENI3_GAMMA (Ni)0.744(Ge)0.256
GRAPHITE (B,C)1
HCP_A3: > Metallic HCP_A3 solution, alpha_Mg/Hf/Sc/Ti/Zr, epsilon_CuZn, etc. (Ag,Mo,Be,Nb,Hf,Sc,Ti,Mn,La,Cu,Zr,Ni,Er,Ca,In,Ga,K,Ce,Bi,Co,Li,Y,Ge,Sr,Cr,Si,V,Al,Zn,Mg,Sn,Na,Fe,Cd,Pb)1(C,Va,B,H)0.5
HCP_CA (Ca)1(Va,H)0.5
HF2SI (Hf)0.6666667(Si)0.3333333
HF3SI2 (Hf)0.6(Si)0.4
HF5SI3 (Hf)0.625(Si)0.375
HF5SI4 (Hf)0.555556(Si)0.444444
HFMN (Hf)0.5(Mn)0.5

Phase Models
HFSI2 (Hf)0.333333(Si)0.666667
HFSI_OP8 (Hf)0.5(Si)0.5
HIGH_SIGMA (Mn)8(Cr)4(Cr,Mn)18
KNA2 (K)1(Na)2
KZN13 (K)1(Zn)13
L10_TETRA (Cu,Al,Ni,Ti,Mn,Nb)0.5(Ti,Cu,Mn,Nb,Ni,Al)0.5
L12_FCC: > L12 phase, Ni3Si_rt, AlZr3, GeNi3, TiZn3, VZn3 (Al,Ge,Ti,Ni,V)1(Al,Zn,Zr,Ni,Fe)3
LA2NI3 (La)2(Ni)3
LA2NI7_HT (La)2(Ni)7
LA2NI7_LT (La)2(Ni)7
LA2ZN17 (La)0.105(Zn)0.895
LA3NI (La)3(Ni)1
LA3SI2 (La)0.6(Si)0.4

Phase Models
LA3ZN22 (La)0.12(Zn)0.88
LA5SI3 (La)0.625(Si)0.375
LA5SI4 (La)0.5556(Si)0.4444
LA7NI16 (La)7(Ni)16
LA7NI3 (La)7(Ni)3
LAH3 (La)0.25(Va,H)0.5(H,Va)0.25
LANI3 (La)1(Ni)3
LANI5 (La)1(Ni)5
LANI_OC8 (La)1(Ni)1
LASI2_A1 (La)0.36(Si)0.64
LASI2_A2 (La)0.3333(Si)0.6667
LASI_OP8 (La)0.5(Si)0.5
LAZN11 (La)0.083(Zn)0.917

Phase Models
LAZN13 (La)0.071(Zn)0.929
LAZN2 (La)0.333(Zn)0.667
LAZN4 (La)0.2(Zn)0.8
LAZN5 (La)0.1667(Zn)0.8333
LI12SI7 (Li)12(Si)7
LI13SI4 (Li)13(Si)4
LI22SI5 (Li)22(Si)5
LI2ZN3_H (Zn,Li)2(Li,Zn)3
LI2ZN3_L (Li)2(Li,Zn)3
LI2ZN5_H (Zn,Li)2(Zn)5
LI2ZN5_L (Zn,Li)2(Zn)5
LI7SI3 (Li)7(Si)3
LIQUID: > Metallic LIQUID solution phase (Zr,Mg2Ge,Be,Sr,P,Mn,Bi,Ce,Ti,Ga,Cr,Si,La,Ca,Er,Hf,Cu,Mg,In,Sc,Ni,Ge,Co,Mo, Li,Ag,K,V,H,Al,Cd,C,Na,Mg2Sn1,B,Y,Sn,Pb,Nb,Zn,Lih,Fe,Zn2Zr)1

Phase Models
LIZN2 (Li)1(Zn)2
LIZN4_H (Zn,Li)0.2(Li,Zn)0.8
LIZN4_L (Zn,Li)1(Li,Zn)4
M11GE8_OP76: > Cr11Ge8, V11Ge8 (Cr,V)0.579(Ge)0.421
M23C6_D84: > Cr23C6, Mn23C6, Mn23SC6 (Mn,Cr)23(Sc,C)6
M3B4_D7B: > V3B4, Ti3B4, Mn3B4, Cr3B4 (B)4(Mn,Ti,V,Cr)3
M5C2 (Mn)5(C)2
M7C3_D101: > Cr7C3, Mn7C3 (Mn,Cr)7(C)3
MG10NI55SI35 (Mg)2(Ni)11(Si)7
MG12CE (Al,Mg)12(Ce)1
MG17CE2 (Mg)17(Ce)2
MG17SR2 (Mg)17(Sr)2
MG23SR6 (Mg)23(Sr)6

Phase Models
MG24R5 (Mg,Er)5(Mg,Al)24
MG2C3 (Mg)2(C)3
MG2NI16SI11 (Mg)1(Ni)8(Si)5.5
MG2NI3SI (Mg)2(Ni)3(Si)1
MG2NI_HP18 (Mg,Zn)2(Ni,Zn,Cu)1
MG2SI_C1: > solution phase of Mg2Si, GeMg2, Mg2Sn (Mg)2(Si,Ge,Sn)1
MG2SR (Mg)2(Sr)1
MG2ZN3 (Mg)2(Al,Zn,Cu)3
MG38SR9 (Mg)38(Sr)9
MG3CE (Mg)3(Ce,Mg)1
MG41CE5 (Mg)41(Ce)5
MG5NI9SI (Mg)1(Ni)1.8(Si)0.2
MG6MN3NI (Mg)0.5(Mn)0.1666667(Ni)0.33333333

Phase Models
MG7ZN3 (Mg)51(Zn)20
MG9NI29SI16 (Mg)9(Ni)29(Si)16
MGB4 (Mg)1(B)4
MGB7 (Mg)1(B)7
MGC2 (Mg)1(C)2
MGCE (Al,Mg)1(Ce)1
MGH2 (Mg)1(H)2
MGNI6SI6 (Mg)1(Ni)6(Si)6
MGNI6ZN6 (Zn,Mg)3(Zn,Ni,Mg)4(Ni)1(Zn)2
MGZN (Mg)12(Zn,Cu,Al)13
MN11SI19 (Mn)11(Si,Al)19
MN15NI45SI40: > Mn-Ni-Si ternary phase, T1 or N (Mn)0.15(Ni)0.45(Si)0.4
MN15NI50SI35: > Mn-Ni-Si ternary phase, T2 or PHI (Mn)0.15(Ni)0.5(Si)0.35

Phase Models
MN1NI1SI1: > Mn-Ni-Si ternary phase, T4 or E (Mn)1(Ni)1(Si)1
MN2B_D1F (Mn)0.6707(B)0.3293
MN2NISI: > Mn-Ni-Si ternary phase, T8 or S (Mn,Ni)3(Si)1
MN2SN: > Mn(2-x)Sn (Mn)0.643(Sn)0.357
MN3NI2SI: > Mn-Ni-Si ternary phase, T7 or Omega (Mn)3(Ni)2(Si)1
MN3SI (Ni,Fe,Mn)3(Si,Al)1
MN3SN2 (Mn)3(Sn)2
MN3TI (Mn)3(Ti)1
MN4TI (Mn)0.815(Ti)0.185
MN52NI29SI19: > Mn-Ni-Si ternary phase, T11 or W (Mn)0.52(Ni)0.29(Si)0.19
MN5SI3_D88: > Mn5Si3, Cr3Si5, Fe5Si3, Ge3Mn5, Ge3Zr5, Si3Zr5, Sn3Ti5 (Ni,Fe,Cr,Zr,Ti,Cu,Mn)5(Cr,Al,Sn,Si,Ge)3
MN66NI4SI30: > Mn-Ni-Si ternary phase, T10 or U (Mn)0.66(Ni)0.04(Si)0.3
MN6NI16SI7: > Mn-Ni-Si ternary phase, T3 or G (Mn)0.206897(Ni)0.551724(Si)0.241379

Phase Models
MN6NISI3: > Mn-Ni-Si ternary phase, T9 or R (Mn)0.61(Ni)0.12(Si)0.27
MN6SI (Mn,Al)17(Zn,Si)3
MN7NI7ZN86 (Mn)0.07(Ni)0.07(Zn)0.86
MN9SI2 (Mn)33(Si)7
MNB4 (Mn)0.2(B)0.8
MNNI2 (Ni,Mn)1(Ni)2
MNNISI_T5: > Mn-Ni-Si ternary phase, T5 or "tao 1" (Mn)1(Si,Ni)2
MNNISI_T6: > Mn-Ni-Si ternary phase, T6 or "tao 2" (Mn)1(Si,Ni)2
MNSC4 (Mn)0.2(Sc)0.8
MNTI_HT (Mn)0.515(Ti)0.485
MNTI_LT (Mn)1(Ti)1
MNV_SIGMA (V,Mn)10(V)4(V,Mn)16
MNZN9 (Mn)0.1(Zn)0.9

Phase Models
MO5SI3 (Mo)0.5(Si,Mo)0.125(Al,Mo,Si)0.375
MOSI2 (Si,Al)2(Mo)1
NASI_HT (Na)1(Si)1
NASI_LT (Na)1(Si)1
NAZN13 (Na)1(Zn)13
NI10HF7 (Ni)0.588(Hf)0.412
NI10ZR7 (Ni)23(Zr)17
NI11HF9 (Ni)0.55(Hf)0.45
NI11ZR9 (Ni)11(Zr)9
NI21HF8 (Ni)0.724(Hf)0.276
NI21ZR8 (Zr)8(Ni)21
NI2SIZN3_T3 (Ni)2(Si)1(Zn)3
NI2SIZN_T1 (Ni)0.5(Si)0.25(Zn)0.25

Phase Models
NI2SI_HT (Cu,Ni)1(Va,Ni)1(Si,Al)1
NI2V1 (Ni)2(V)1
NI2V7 (Ni)2(V)7
NI3HF_HT (Ni)0.75(Hf)0.25
NI3HF_LT (Ni)0.75(Hf)0.25
NI3SI2 (Ni,Fe)3(Si)2
NI3SI_HT (Ni,Fe)3(Al,Si)1
NI3SI_MT (Si)1(Ni)3
NI3SN2_HT (Ni)0.33333(Sn,Ni)0.33334(Sn)0.33333
NI3SN2_LT (Sn)0.2(Ni,Sn)0.4(Ni)0.4
NI3SN4 (Ni)0.25(Ni,Sn)0.25(Sn)0.5
NI3SN_D019: > Ni3Sn, SnTi3, SnMn3, AlLa3 (Sn,Al,Va,Ge)1(Ni,Mn,Fe,La,Ti)3
NI3SN_HT (Ni,Sn)0.25(Sn,Ni)0.25(Ni)0.5

Phase Models
NI3TI_D024 (Ti,Ni)0.75(Ni,Ti)0.25
NI4B3_MONO (Ni)0.564(B)0.436
NI4B3_ORTH (Ni)0.586(B)0.414
NI5HF (Ni)0.833(Hf)0.167
NI5SI2 (Ni,Cu,Fe)5(Si,Al)2
NI7HF2 (Ni)0.778(Ni,Hf)0.222
NI7HF3 (Ni)0.7(Hf)0.3
NI7SC2 (Sc)0.222222(Ni)0.777778
NI7ZR2 (Ni)7(Zr)2
NI9SI2ZN_T2 (Ni)0.75(Si)0.1675(Zn)0.0825
NIHF2 (Ni,Va)1(Hf)2
NIHF_HT (Ni)0.5(Hf)0.5
NIHF_LT (Ni)0.5(Hf)0.5

Phase Models
NISC2 (Sc)0.72(Ni)0.28
NISC_B2 (Sc)1(Ni)1
NISI2 (Zn,Cu,Al,Si)2(Ni,Mn,Fe,Cu)1
NISIZN_T4: > Ni-Si-Zn tao 4, Ni3Si2Zn1 (Ni)3(Si)2(Zn)1
NISI_B31: > GeNi, NiSi (Ni,Fe)1(Zn,Si,Ge)1
NISR (Ni)0.5(Sr)0.5
NITI2 (Ni,Ti)1(Ni,Ti)2
NIZN8 (Ni)0.1111111(Mn,Al,Zn)0.8888889
NIZN_LT (Mn,Si,Fe,Ni,Zn,Al)0.5(Si,Mg,Fe,Ni,Mn,Al,Zn)0.5
O1_DIS: > The disordered O phase (Nb,Al,Ti)0.75(Nb,Al,Ti)0.25
ORD_L12: > Ordered L12, having Gibbs energy contribution from DISO_A1 (Sc,Sn,Cr,K,Mn,Ni,La,Ce,Zn,Zr,Mo,Sr,Na,Ge,Co,Mg,Pb,In,Fe,Bi,Ga,Al,Cu,Be,Hf,Cd,Ag,V,Er,Ti,Si,Ca,Li)0.75 (Ge,Ti,Bi,K,Mo,Cd,Sc,Pb,Cu,Si,Ga,Fe,Ag,Ca,Zr,Co,Ce,Zn,Sn,Mn,Hf,La,Mg,In,Ni,Be,Er,Na,Li,Cr,V,Al,Sr)0.25(Va)1
ORTHORHOMBIC_GA (Ga)1
O_PHASE: > The O phase (Nb,Ti)0.5(Nb,Ti,Al)0.25(Ti,Nb)0.25

Phase Models
P2ZN3_HT (P)2(Zn)3
P2ZN3_LT (P)2(Zn)3
P2ZN_HT (P)2(Zn)1
P2ZN_LT (P)2(Zn)1
QPRIME: > Coherent / semi-coherent version of Q_ALCUMGSI (Al)5(Cu)2(Mg)8(Si)6
Q_AL7CU3MG6: > Al7Cu3Mg6, Al-Cu-Mg ternary phase, aka. Q_AL7CU3MG6 (Al)7(Cu)3(Mg)6
Q_ALCUMGSI: > Quaternary phase, aka Q, Al5Cu2Mg8Si6, Al3Cu2Mg9Si7 & Al4Cu2Mg8Si7 (Al)5(Cu)2(Mg)8(Si)6
RED_P (P)1
RHOMBO_A7 (Sn,Bi,In)1
SC13ZN58 (Sc)0.1831(Zn)0.8169
SC1ZN1 (Sc)0.5(Zn)0.5
SC3SI5_HT (Sc)0.375(Si)0.625
SC3SI5_LT (Sc)0.375(Si)0.625

Phase Models
SC3ZN17 (Sc)0.15(Zn)0.85
SC5SI3 (Sc)0.625(Si)0.375
SCSI (Sc)0.5(Si)0.5
SCZN12 (Sc)0.077(Zn)0.923
SCZN2 (Sc)0.3333(Zn)0.6667
SI2SR_HT (Va,Si)2(Sr)1
SI2SR_LT (Si)2(Sr)1
SI2TI_C54: > Ge2Ti, Si2Ti, Sn2Zr (Sn,Si,Al,Ge)2(Zr,Ti)1
SI2ZR3_D5A: > Si2Zr3, B2V3 (Si,B)2(Zr,V)3
SI2ZR_C49: > Si2Zr, Ge2Zr (Si,Ge)2(Zr)1
SI3TI5_D88 (Si)3(Ti)5
SI4ZR5_TP36: > Si4Zr5, Si4Ti5, Ge4Zr5 (Si,Ge)4(Ti,Zr)5
SIB3 (B)6(Si)2(Si,B)6

Phase Models
SIB6 (B)210(Si)23(Si,B)48
SIBX (B)61(Si)1(Si,B)8
SIC (C)1(Si)1
SIGMA (Mn,Fe,Ni)8(Cr,V)4(V,Fe,Cr,Ni,Mn)18
SIP2 (Si)1(P)2
SIP_OC48 (Si)1(P)1
SIZR3_TP32: > SiZr3, SiTi3, GeZr3 (Si,Ge)1(Zr,Ti)3
SN3TI2 (Sn)3(Ti)2
SN3ZR5: > aka eta (Zr)5(Sn)3(Sn,Va)1
SN5TI6_OI44: > Sn5Ti6, Si5V6, Ge5Ti6 (Ge,Sn,Si)5(Ti,V)6
SNZR3_A15 (Zr,Sn)3(Zr,Sn)1
SN_HP1 (Sn,Cd,In)1
SR3SN5 (Sr)0.375(Sn)0.625

Phase Models
SRB6 (Sr)1(B)6
SRSN3 (Sr)0.25(Sn)0.75
SRSN4 (Sr)0.2(Sn)0.8
SRZN5_LT (Sr)1(Zn)5
S_DPRIME: > metastable precipitate, related to S_PHASE (Al)5(Cu)5(Mg)2
S_PHASE: > aka Al2CuMg or S (Si,Al)2(Cu)1(Mg)1
S_PRIME: > slightly distorted S_phase. Strain & interfacial energy need to added (Al)2(Cu)1(Mg)1
TETRA_A6 (Sn,In)1
TET_A6P (In,Sn)1
THETA_DPRIME (Al)3(Cu)1
THETA_PRIME (Al)2(Cu)1
TIZN10 (Ti)1(Zn)10
TIZN15 (Ti)1(Zn)15

Phase Models
TIZN2 (Ti)1(Zn)2
TIZN5 (Ti)1(Zn)5
T_PHASE: > Solution (Al,Cu,Zn)49Mg32, stable in Al-Mg-Zn, Al-Cu-Mg, Al-Cu-Mg-Zn (Mg)26(Al,Mg)6(Zn,Mg,Cu,Al)48(Al)1
T_PRIME: > metastable precipitate, related to T_PHASE (Al)0.3(Mg)0.45(Zn)0.25
U1_AL2MGSI2: > metastable precipitate, U1_Al2MgSi2, Al-containing Pre-beta phase (Al)2(Mg)1(Si)2
U2_AL4MG4SI4: > metastable precipitate, U2_Al4Mg4Si4, Al-containing Pre-beta phase (Al)1(Mg)1(Si)1
V17GE31 (V)0.354(Ge)0.646
V2B3 (V)0.4(B)0.6
V2ZR (V)2(Zr)1
V3C2 (V)3(C)2
V3GE (V)0.75(Ge)0.25
V3SI (V,Si)0.75(V,Si)0.25
V3SN (Sn)0.205(V)0.795

Phase Models
V4ZN5 (V)4(Zn)5
V5B6 (V)0.454545(B)0.545455
VSN2 (Sn)0.6(V)0.4
V_PHASE: > solution of Mg2Zn11, Al5Cu6Mg2; aka Z (Zn,Si,Al)5(Zn,Cu)6(Mg)2
WHITE_P (P)1
ZN13M2 (Fe,Ni)1(Zn)6.5
ZN22ZR (Zn)22(Zr)1
ZN2ZR (Zn)2(Zr)1
ZN39ZR5 (Zn)39(Zr)5
ZN3ZR_HT (Zn)3(Zr)1
ZN3ZR_LT (Zn)3(Zr)1
ZRB12 (B)12(Zr)1
ZRM5_C15B: > Cu5Zr, Ni5Zr (Ni,Cu)5(Zr)1

TCAL7 Properties Data

In this section:

Electrical Resistivity and Thermal Conductivity Models

The TCS Al-based Alloy Database (TCAL) database includes electrical resistivity and thermal conductivity properties data.

All binary systems are modeled by using experimental data or theoretical estimations. Ternary and multicomponent systems can be extrapolated and the calculation results agree very well with the measurements in the selected case studies.

Electrical Resistivity Model Description

The semi-empirical model for electrical resistivity is built based on the Matthiessen's rule [1997, De-Bruyn-Ouboter]. In general, the electrical resistivity of a metallic alloy consists of residual resistivity (ρ_0) and electron-phonon resistivity (ρ_{e-p}), as well as magnetic resistivity (ρ_m). The residual resistivity is due to the scatterings of impurities and defects that exist in well-annealed and high purity alloys, and the value of ρ_0 is generally considered independent of temperature.

[*Eq. 1*] $$\rho = \rho_0 + \rho_{e-p} + \rho_m$$

ρ_{e-p} is described with the modified Bloch-Grüneisen equation [1928, Bloch; 1933, Grüneisen] and corrections can be made in cases where other types of scatterings play considerable roles.

[*Eq. 2*] $$\rho_{e-p} = A \cdot \left(\frac{T}{\theta_R}\right)^5 \cdot J_5\left(\frac{\theta_R}{T}\right)$$

[*Eq. 3*] $$A = \frac{\frac{3}{2}hq_D^6(G')^2}{4e^2(m^*)^2 n_c k_B \theta_D k_F^2 \nu_F^2}$$

[*Eq. 4*] $$J_n\left(\frac{\theta_D}{T}\right) = \int_0^{\frac{\theta_D}{T}} \frac{x^n e^x}{(e^x-1)^2} dx$$

The characteristic temperature θ_R plays a similar role and is also approximated as the Debye temperature (θ_D), which can be readily obtained from low-temperature heat capacity and elastic constants data as well as theoretical computations. The approximation of θ_R as θ_D indicates that transverse phonons play a role in electron scattering. k_F is the electron wave number at the Fermi surface. q_D is the phonon Debye wave number. h is the Planck constant. G' is a constant representing the strength of the e-p interaction and cannot be easily estimated. m^* is the electron effective mass. n_c is the number of unit cells per unit volume. v_F is the electron velocity at the Fermi surface.

To describe the drastic change of the magnetic resistivity (ρ_m) around the Curie (or Neel) temperature, T_C, of a magnetic alloy, an empirical model is proposed using the dimensionless temperature T/T_C and a parameter ρ_{spd} that stands for the resistivity due to spin disordering. According to this model, Eq. 5, ρ_m approaches

ρ_{spd}, when the temperature is well above T_C, and is 0 when the temperature is far below T_C. ρ_{spd} depends only on composition and is described with the Redlich-Kister (R-K) expression. Apparently, ρ_{spd} has a positive value for magnetic elements, and compounds as well as endmembers, and is 0 for non-magnetic ones.

In a typical binary system made of a magnetic element A and a non-magnetic element B, ρ_{spd} decreases usually from ρ_{spd}^{A} to 0 at a certain composition (x_*). Such a behavior is also seen in magnetic moment and Curie temperature. ρ_{spd} is expected to be zero in the composition range from x_* to element B, and will be forced to zero when the R-K expansion leads inevitably to negative values over this composition range. T_C is available from the thermodynamic description in the database.

[*Eq. 5*]
$$\rho_m = \rho_{spd} \cdot \left(1 - e^{\left(-\frac{3}{2}\left(\frac{T}{T_c}\right)^3\right)}\right)$$

The semi-empirical model (as given in Eq. 1 to Eq. 5) is first fitted to experimental data. The description is then extrapolated to a wider temperature range if necessary, either to extreme temperatures where the structure is no longer stable or to where experimental data are missing. Polynomials are then derived with the experimental data, together with the extrapolated values, and stored in the database. The model as given in Eq. 5 is implemented in Thermo-Calc, so the magnetic contribution can be excluded from the polynomials and separately modeled, and it will be automatically included during the calculations.

Thermal Conductivity Model Description

Experimental data of thermal conductivity are used to derive descriptions in polynomials, which are stored in the database, despite that it consists of two components, electronic thermal conductivity (κ_e) and lattice thermal conductivity κ_g. In other words, they are not separately treated.

In cases where experimental data are absent or sparse, however, κ_e and κ_g can be separately predicted and summed up to give the total thermal conductivity. κ_e can be predicted from ρ or vice versa, by employing the Wiedemann-Franz Law [1853, Franz; 1985, Jones], respectively, to the residual resistivity, magnetic resistivity and intrinsic resistivity.

[*Eq. 6*]
$$\frac{1}{\kappa_e} = W_e = \frac{\rho_0 + \rho_m + \rho_i}{L_0 T}$$

L_0 is known as the Sommerfeld value of the Lorenz number, $2.4453 \times 10^{-8} W\Omega/K^2$

[*Eq. 7*]
$$\rho_i = \frac{A}{L_0 T} \cdot \left(\frac{T}{\theta_R}\right)^5 \cdot J_5\left(\frac{\theta_R}{T}\right) \cdot f$$

$$f = 1 + \frac{3}{\pi^2} \cdot \left(\frac{k_F}{q_D}\right)^2 \cdot \left(\frac{\theta_R}{T}\right)^2 - \frac{1}{2\pi^2} \cdot \frac{J_7\left(\frac{\theta_R}{T}\right)}{J_5\left(\frac{\theta_R}{T}\right)}$$

[*Eq. 8*]

The intrinsic resistivity (ρ_i) is based on Eq. 2 for the e-p processes, but corrections are provided, as given in Eq. 8: the first term corresponds to large-angle scattering that satisfies the original Wiedemann-Franz Law; the second one is due to inelastic small-angle (vertical processes) and has no counterpart in the electrical resistivity; the third term is a correction that accounts for situations where large-angle scattering can reverse the electron direction without actually assisting to restore the distribution back to equilibrium.

κ_g can be predicted with the Slack model in a temperature range where only anharmonic Umklapp phonon-phonon interactions are important. In other words, normal processes are neglected as a first approximation [2002, Morelli; 1979, Slack]. The most reasonable version among several ones is given below [1965, Julian].

$$\kappa_p^U = A' \cdot \frac{M_a \cdot \theta_D^3 \cdot \delta}{\gamma^2 \cdot n_c^{\frac{2}{3}}} \cdot \frac{1}{T}$$

[*Eq. 9*]

$$A' = \frac{2.43 \cdot 10^{-5}}{1 - \frac{0.514}{\gamma} + \frac{0.228}{\gamma^2}}$$

[*Eq. 10*]

The Debye temperature, θ_D can be obtained from low-temperature heat capacity or elastic constant data. M_a is the average atomic mass, δ^3 the volume per atom, n_c the number of atoms in a unit cell, and γ the Grüneisen coefficient. A typical value for A' is evaluated to be 3×10^{-5} using $\gamma = 2$ as the Grüneisen coefficient, and can be used in the absence of experimental information. It can also be obtained from e.g. DFT calculations of elastic properties.

Model Parameters

The extended TDB format accepts parameters describing electrical resistivity and thermal conductivity, together with spin disordering resistivity. Examples for unary and binary systems are given below:

```
ELRS(FCC_A1,AL:VA;0)
ELRS(FCC_A1,AL,CO:VA;0)
THCD(FCC_A1,AL:VA;0)
THCD(FCC_A1,AL,CO:VA;0)
ESPD(FCC_A1,CO:VA;0)
ESPD(FCC_A1,AL,CO:VA;0)
```

Calculation and Plot Variables

- `ELRS` – Electrical resistivity
- `ELCD` – Electrical conductivity
- `THCD` – Thermal conductivity
- `THRS` – Thermal resistivity
- `THDF` – Thermal diffusivity

All the above quantities can be calculated, retrieved, shown and plot in Thermo-Calc via the variables in the Console Mode or via the quantity names in the Graphic Mode (see sections below).

Console Mode

The quantities corresponding to the variables of `ELRS`, `ELCD`, `THCD`, `THRS` and `THDF` can be calculated in Console Mode for a phase, e.g. `ELRS(FCC_A1)`, or for a system, i.e. `ELRS`. The results can be shown in the POLY module with the command SHOW_VALUE or illustrated as a plot in the POST module with the command PLOT_DIAGRAM.

Graphical Mode

On the **Plot Renderer** in Graphical Mode, electrical resistivity, electrical conductivity, thermal conductivity, thermal resistivity, and thermal diffusivity can be selected from the axes lists, tabulated and plotted using the quantity names, with options for a specific phase, all phases or for a system.

TC-Python

The quantities of `ELRS`, `ELCD`, `THCD`, `THRS` and `THDF` can be retrieved, for a phase, e.g. `ELRS(FCC_A1)`, or for a system, i.e. `ELRS`, via `get_value_of()` or `get_values_of()`, from most phase equilibrium calculations in TC-Python, for instance,

- `with_single_equilibrium_calculation()`,
- `with_property_digram_calculation()` or
- `with_batch_equilibrium_calculation()`.

Surface Tension of Metallic Liquid Alloys Model

The TCS Al-based Alloy Database (TCAL) database includes surface tension of metallic liquid alloys properties data.

All the surface tension of all elements and binary systems are assessed.

Model Description

The chosen model for the surface tension of metallic liquid alloys is the modified Guggenheim model [2019, Vermot des Roche]:

$$\sigma(x_i^B,T) = -\frac{RT}{S(x_i^B,T)}\ln\left[x_1^B \exp\left(-(1+\Xi_1 \cdot x_2^S(x_i^B,T))\frac{\sigma_1(T)S_1(T)}{RT}\right) + x_2^B \exp\left(-(1+\Xi_2 \cdot x_1^S(x_i^B,T))\frac{\sigma_2(T)S_2(T)}{RT}\right)\right]$$

where

- x_i^B is the bulk composition
- σ_i is the surface tension
- S and S_i are the total and the partial molar surface of species i defined as

$$S_{(i)} = 1.901 \cdot N_A^{1/3} \cdot V_{m,(i)}^{2/3}$$

- N_A being the Avogadro number and $V_{m,(i)}$ the molar volume of the system or the species i.
- x_i^S is the composition of i in surface, which is a function of bulk composition and T and defined as follows:

$$x_i^{S,id}(x_i^B,T) = \frac{x_i^B}{x_i^B + x_j^B \exp\left(\frac{S(x_i^B,T)[\sigma_i(T)-\sigma_j(T)]}{RT}\right)}$$

- Ξ_1 and Ξ_2 are called damping factors and these parameters are fitted for species 1 and 2 of binary systems.

The extrapolation to higher-order systems is straightforward. The ideal surface composition for a multicomponent system is:

$$x_i^{S,id}(T,x_i^B,x_j^B,\dots) = \frac{x_i^B}{x_i^B + \sum_{j\neq i} x_j^B \exp\left(\frac{S_{ij}(x_i^B,T)\cdot[\sigma_i(T)-\sigma_j(T)]}{RT}\right)}$$

and the surface tension of a multicomponent alloy is obtained from:

$$\sigma(T, x_i^B, x_j^B, \dots) = -\frac{RT}{S(T, x_i^B, x_j^B, \dots)} \cdot \ln\left[\sum_{i=1}^{n}\sum_{j\neq i} x_i^B \exp\left(-(1 + x_j^S(T, x_i^{B,ij}) \cdot \Xi_i^{ij})\frac{\sigma_i(T) S_i(T)}{RT}\right)\right]$$

Reference

[2019, Vermot des Roche] M. Vermot des Roches, A. E. Gheribi, P. Chartrand, "A versatile multicomponent database for the surface tension of liquid metals," Calphad. 65, 326–339 (2019).

Corresponding Variables

The corresponding variable for surface energy of pure elements is SIGM. For instance, the surface tension of pure A is written as SIGM(LIQUID,A;0). The corresponding X_1 and X_2 parameters for A-B binary system are respectively written as following:

```
PARAMETER XI(LIQUID,A,B:0)
PARAMETER XI(LIQUID,A,B:1)
```

The surface energy of the liquid is accessed via SURF(LIQUID).

Plot Variables

Console Mode

The surface energy can be calculated through step calculations in Console Mode. The plot variable is `SURF(LIQUID)`.

Graphical Mode

The surface energy is calculated using the **One-axis calculation** type in Graphical Mode. The corresponding plot variable is *Surface tension*.

TC-Python

In TC-Python, it can be plotted using `property-diagram_calculation()` or `with_batch_equilibrium_calculation()`. The plot variable is `SURF(LIQUID)`.

Graphical Mode and Console Mode Examples

There are two basic examples included with your software installation and that use demonstration

(DEMO) databases.

Search the help (press F1 when in Thermo-Calc) for brief descriptions of these examples, or browse to the examples located in your installation. From the main menu, **Help→ Examples Files**:

- Graphical Mode **T_11_Surface_tension_in_Cu-Zr.tcu**
- Console Mode `tcex56`

Viscosity of the Metallic Liquids Model

The TCS Al-based Alloy Database (TCAL) database includes viscosity of the metallic liquids properties data.

Model Description

The viscosity of metallic liquid alloys is modeled as follows:

$$RT \ln \eta = RT \ln \eta_0 + E$$

where

- η is the dynamic (or shear) viscosity of the liquid,
- η_0 is the viscosity at finite temperatures,
- E is the activation energy in J/mole,
- R is the gas constant, and
- T is the absolute temperature.

The SI unit of viscosity is pascal.second (Pa.s). The viscosity parameters are expanded via Redlich-Kister polynomials.

For example, viscosity of a liquid A-B alloy is:

$$\begin{aligned} RT \ln \eta_{alloy} = {} & x_A (E_A \cdot RT \ln \eta_0^A) \\ & x_B (E_B \cdot RT \ln \eta_0^B) \\ & x_A x_B (L_0 + (x_A - x_B) \cdot L_1) \end{aligned}$$

The two first terms are the contributions for the end-members, A and B elements and the last term accounts for the excess viscosity. Basically, the activation energies are optimized. L_0 and L_1 etc. are the parameters that are optimized to fit the viscosity data.

The kinematic viscosity, η is the ratio of the dynamic viscosity to the density, ρ, of the alloy:

$$\nu = \eta / \rho$$

The SI unit of kinematic viscosity is square meter per second (m^2/s).

Corresponding Variables

In Console Mode, the viscosity can be plotted via a step calculation vs. temperature or composition. The calculated property in Thermo-Calc is VISC of the liquid phase. The calculated VICS property is not the

viscosity (η) but is related to η via $RT\ln(\eta)$, thus in order to plot the viscosity or η you define a function for η as follows:

$$\eta = \exp(VISC(LIQUID)/RT)$$

The default unit is Pa.s.

However, it is also possible to directly get the values for dynamic and kinematic viscosity in Console Mode and using TC-Python. The relevant properties are DVIS (dynamic viscosity) and KVIS (kinematic viscosity). For example, once the equilibrium is calculated in Console Mode, one can get the viscosity value by:

`show DVIS(liq)` or `show KVIS(liquid)`.

In Graphical Mode, the viscosity (η) is directly plotted when using the One-axis calculations available with various calculators.

Graphical Mode and Console Mode Examples

There are two basic examples included with your software installation and that use demonstration (DEMO) databases.

Search the help (press F1 when in Thermo-Calc) for brief descriptions of these examples, or browse to the examples located in your installation. From the main menu, **Help→ Examples Files**:

- Graphical Mode **T_12_Viscosty_in_Cr-Ni.tcu**
- Console Mode `tcex55`

Molar Volume Model

The TCS Al-based Alloy Database (TCAL) includes molar volume properties data.

Molar volume can be used to establish a connection with some significant physical properties, for example, viscosity, electrical conductivity and surface tension. It is the reciprocal of density multiplied by molar mass.

Model Description

The model used to describe the molar volume at ambient pressures is:

$$V_m(T) = V_0 exp(\int_{T_0}^{T} 3\alpha dT)$$

A simple polynomial is used to model non-magnetic volumetric expansivity above 298K:

$$3\alpha = a + bT + cT^2 + dT^3 + eT^{-2}$$

The model described above is implemented in Thermo-Calc software with two parameters, V0 and VA, and α is the linear thermal expansivity at 1 bar and 3α is the volumetric thermal expansivity.

Molar Volume Descriptions

Parameter	Unit	Description
V0 (phase, constituent array)	m^3/mol	Volume at 1 bar and reference temperature T0
VA (phase, constituent array)	None	$\int_{T_0}^{T} 3\alpha dT$

TCAL: TCS Aluminium-based Alloys Database Revision History

Current Database Version

Database name (acronym):	**TCS Al-based Alloy Database (TCAL)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**7.0**

Changes in the Most Recent Database Release

TCAL6 to TCAL7

Software release 2020b (June 2020)

New Thermophysical Properties

- Electrical resistivity is modeled for crystalline phases and liquid. The descriptions can be used for deriving electrical conductivity.
- Thermal conductivity is modeled for crystalline phases and liquid. The descriptions can be used for deriving thermal resistivity as well as thermal diffusivity (by combining with our density and heat capacity data).
- Viscosity and surface tension of liquid are modeled.

New Elements and Systems

- Added new minor-alloying elements: Nb, P and Y.
- Al-P, P-Si, P-Zn, Al-P-Si, and Al-P-Zn are modeled. The systems help to predict the formation of the ALP phase in aluminum alloys and to interpret its impacts on the microstructure modification.
- Al-Nb, as well as Nb-Ti and Al-Nb-Ti, is modeled for the minor-alloying element Nb.
- Al-Y, as well as Ti-Y and Al-Ti-Y, is modeled for the minor-alloying element Y.
- Six more Al-containing ternary systems are modeled, Al-C-Cr, Al-C-Mg, Al-C-V, Al-Cr-Mg, Al-Mg-Ti, and Al-Si-Sr, to make the Al-rich multi-component description more complete.

New Metastable Phase

- The semi-coherent version of the quaternary Q_ALCUMGSI phase is modeled as a metastable phase, QPRIME. It is expected to be used in precipitation simulations.

Updated Systems and Phases

- Al-C is updated taking into account the most recent modeling work.
- Si-Sr is updated and now reproduces the most recent modeling work.
- Al-C-Si is updated with the improved Al-C binary description.
- Al-Sc-Si is updated by modeling the Si solubility in the AL3X (Al3Sc-based) phase, which is a strengthening precipitate in some aluminum alloys
- Al-Fe-Mg-Si: the quaternary phase π-AL18FE2MG7SI10 is refined to make better predictions for solidification and lower-temperature heat treatments of related aluminum alloys.
- Al-Fe-Mn-Si is updated by modeling the Mn solubility in AL8FE2SI.
- Cr and Mo are introduced to the Al15Si2M4 (M = Cr, Fe, Mn and Mo) phase, which is of industrial importance in Al-Mn-Si and Al-Fe-Mn-Si based alloys.

Previous Releases

TCS Aluminium-based Alloys Database version 1 (TCAL1) was originally released in 2011.

TCAL5.1 to TCAL6

Software release 2019a (December 2018).

- Added a new element Mo, the Al-Mo and Mo-Si binary systems, and the Al-Mo-Si ternary system
- FCC_A1 is now independently modeled and no longer coupled with FCC_L12. The FCC_L12 phase modeled with the partitioning model is now separated and named as ORD_L12.
- Updated the Al-Cu-Mg-Zn metastable precipitates of industrial importance: S_prime and T_ prime are remodeled; S_DPrime is newly modeled; especially, the Eta_prime phase is remodeled by considering the Cu solubility.

TCAL5 to TCAL5.1

Software release version: 2018b (June 2018)

Updates to the following systems:

- Al_6(Cu, Fe, Mn) remodeled in Al-Cu-Fe-Mn and treated as a metastable phase in Al-Cu-Fe
- Improved description of Al_7Cu_2Fe
- Updated Si-Ti and Al-Si-Ti
- Improved volume description

TCAL4 to TCAL5

Software release version: 2017b (October 2017)

This update highlights the assessment of 18 binary systems and 25 ternary systems relevant to the 8xxx and 8xx.x series of industrial aluminum alloys, including but not limited to Al-Ce, Al-Er, Al-Li, Al-Sc, and Al-Sn based alloys.

The rare earth element Er, which may form the L12-type Al3Er stable precipitate in aluminum alloys, was newly added to the database. The Ag-Er, Al-Er, Cu-Er, Er-Fe, Er-Mg, Er-Si and Er-Zr binary systems and the Al-Cu-Er, Al-Er-Fe and Al-Er-Mg ternary systems were assessed.

The Ce-Cr, Ce-Fe, Ce-Mg, Ce-Mn, Ce-Ni and Ce-Si binary systems and the Al-Ce-Cr, Al-Ce-Cu, Al-Ce-Fe, Al-Ce-Mg, Al-Ce-Mn, Al-Ce-Ni and Al-Ce-Si ternary systems were assessed.

The L12 type metastable Al3Li (δ') phase, which is an important strengthening precipitate in some Li-containing aluminium alloys, was modelled. The Al-Li-Zr and Cu-Li-Mg systems were assessed.

The Bi-Sn, Cd-Sn, In-Sn and Sn-Pb binary systems and the Al-Bi-Sn, Al-Cd-Sn, Al-Cr-Sn, Al-Cu-Sn, Al-In-Sn, Al-Sn-Pb, Al-Sn-Si and Al-Sn-Zn ternary systems were assessed.

Sc-Ti, Al-Sc-Si, Al-Sc-Ti, Al-Sc-Zr and Al-Si-Ti were assessed. Ag-Cu was replaced and Ag-Al-Cu was assessed.

TCAL3 to TCAL4

Software release version: 2015a (June 2015)

The metastable Al-Cu precipitate Ω was modeled as the Al2Cu_OMEGA phase. In the Al-Cu-Mg-Zn system, the descriptions of the metastable precipitates ETA_PRIME (η') and T_PRIME (T') were refined. In the Al-Mg-Si system, the BETA_AL_DPRIME (Al-containing β'') phase was merged into BETA_DPRIME (β'') and treated as the same phase.

53 Ag-, H-, Hf-, K-, La-, Li-, Na- and/or Sc-containing binary systems were added, Ag-Cu, Ag-Fe, Ag-La, Ag-Li, Ag-Mg, Ag-Mn, Ag-Na, Ag-Ni, Ag-Si, Ag-Zn, Cu-H, Cu-Hf, Cu-La, Cu-Na, Fe-H, Fe-Hf, Fe-K, Fe-La, Fe-Li, Fe-Na, H-K, H-La, H-Li, H-Mg, H-Mn, H-Na, H-Ni, H-Zn, Hf-K, Hf-Li, Hf-Mg, Hf-Mn, Hf-Na, Hf-Ni, Hf-Sc, Hf-Si, K-Li, K-Mg, K-Na, K-Zn, La-Mn, La-Ni, La-Sc, La-Si, La-Zn, Li-Mn, Li-Na, Li-Sc, Li-Zn, Na-Sc, Na-Si, Na-Zn, and Sc-Zn. The previous Ag-Al binary description was replaced.

HCP_ZN was merged into HCP_A3. Necessary adjustments were made for the descriptions of Zn-containing systems in order to reproduce the phase equilibria.

Zr was introduced to Al3Ti_D022 and Ti to Al3Zr_D023. Al-Ti was updated in the Al-rich region. A preliminary assessment of the Al-Ti-Zr system was conducted. The description of Al4Mn_R in the Al-Fe-Mn system was refined.

Molar volumes and thermal expansivities were evaluated for all the newly added phases and end-members. Some existing volume data were updated as well.

TCAL2.1.1 to TCAL3

Software release version: 4.0 (June 2014)

19 binary systems were added, Ag-Ca, Ca-Cu, Ca-Fe, Ca-H, Ca-La, Ca-Li, Ca-Mn, Ca-Na, Ca-Ni, Ca-Sc, Ca-Si, Ca-Sr, Ca-Zn, Ag-Sc, Fe-Sc, Mn-Sc, Ni-Sc, Sc-Si and Sc-Zr.

Modeling of Al-Cu metastable precipitates: GPI Zones (described as the miscibility gap of fcc_A1), θ''-Al_3Cu (i.e. GPII Zones) and θ'-Al_2Cu.

Modeling of Al-Cu-Mg-Zn metastable phases: S'-Al_2CuMg, T'-$Al_{0.3}Mg_{0.4}Zn_{0.3}$ and η'-$Al_3Mg_{2.5}Zn_{3.5}$.

Modeling of Al-Mg-Si metastable precipitates: β''-Mg_5Si_6 (GPII zones), Al-containing β''-$Al_2Mg_5Si_4$, β'-Mg_9Si_5, U1-Al_2MgSi_2, U2-$Al_4Mg_4Si_4$ and B'-$Al_3Mg_9Si_7$.

Modeling of the metastable Al_mFe phase (modeled as Al_4Fe), which has been observed in some as-cast aluminum alloys such as AA1xxx, AA5128 and A206.

Necessary volume data were assessed for the new phases and newly introduced end-members. The Sn-Zn and Cu-Fe-Ni descriptions were updated. Some known issues were solved.

TCAL2 to TCAL2.1.1

Software release version: 3.1 (December 2013)

The Al-Fe-Mn-Si quaternary description had been systematically refined, including a deep revision of the Al-Fe-Si description and adjustments of the Al-Fe-Mn and Al-Mn-Si descriptions. It has been validated that this refinement improved the phase formation in a wide range of casting and wrought aluminum alloys, since Fe, Mn and Si are the most common additives and/or impurities in aluminum alloys.

A new Al-Ni description had been adopted and adjustments were subsequently made on the Al-Ni-based ternary systems.

The BCC_B2 description in the Ni-Zn binary system was reassessed. The Al-Ni-Zn ternary was reassessed. The Al-Mn-Ni description was improved by solving some known issues.

Both the Al-Cr and Al-V binary systems were improved in the Al-Rich corner. The Al-Si molar volume data were refined.

TCAL1.2 to TCAL2

Software release version: 3.0 (2013).

Since TCAL2, all necessary volume data (including molar volume and thermal expansion) had been added for most of the solution phases and intermetallic phases. This allows for the calculation of volume fraction of phases, as well as density, thermal expansivity and lattice parameters using Thermo-Calc. However, it should be noted that the molar volume data incorporated has no pressure dependence.

21 more binary systems have been implemented: Al-Be, Al-Bi, Al-Cd, Al-Ce, Al-Co, Al-Ga, Al-In, Al-Pb, Bi-Cu, Cd-Cu, Ce-Cu, Co-Li, Cr-Li, Cu-Co, Cu-Ga, Cu-In, Cu-Pb, Cu-Sc, Li-Ni, Li-Si and Li-Zr. Some of them were reassessed in this project. Additionally, the Al-Ca and Al-Sc descriptions have been updated. The $AlLi_2$ phase was considered in Al-Li.

The three ternary systems, Al-C-Si, Al-Cu-Sc, and Al-Li-Si, have been newly implemented. The previous provisional description of the Al-Cr-Si system has been replaced by a much more reliable description, which is derived from a thorough thermodynamic modeling over the entire compositional range and a wide temperature range. The Mn-Ni-Si description is also updated.

TCAL1.1 to TCAL1.2

TCAL1.2 was updated in 2012.

The Cu-Li, Li-Mg, Al-Cu-Li and Al-Li-Mg systems have been assessed and/or implemented in order to be able to predict the phase formation in Al-Cu-Li-Mg(-Zn) alloys (i.e. some of the 2xxx and 8xxx series alloys). The descriptions of the Al-Cu-Mg-Si and Al-Fe-Mn-Si core systems have been refined and validated, in order to give more accurate predictions for commercial Al-based alloys, including wrought alloys from series 2xxx to series 7xxx and foundry alloys series 3xx.x. The Al-Cr-Si system was tentatively assessed to include the Cr-bearing phase $Al_{13}Cr_4Si_4$.

The two compounds, AL8FEMNSI2 and AL5CU2MN3, were removed from the database since their existences were disputed. The VSI2 phase was merged into CRSI2_C40, and the AB3_L12 phase into L12_FCC. Thermodynamic models were reviewed for most phases, and many un-assessed parameters were reasonably estimated. Some phases were renamed to use their conventional names.

Additionally, the C-Mg binary description was reassessed. Now the two Mg carbides, MgC_2 and Mg_2C_3, are metastable and the C solubility in liquid Mg is greatly reduced to accord with the mostly published experimental data.

TCAL1 to TCAL1.1

TCAL1 was released in 2011 and TCAL1.1 was updated in 2012.

The description of the Al-Zn-Mg-Cu-Fe core system has been systematically refined and validated in order to give more accurate predictions for commercial Al-based alloys, especially the 7xxx series alloys. More specifically, crucial corrections or modifications have been made for the following related ternary systems, Al-Cu-Fe, Al-Cu-Mg, Al-Cu-Zn, and Al-Mg-Zn.

Another major enhancement is that users can now get the conventional phase names in Al-based alloys for a general name used in the database by using the command LIST_SYSTEM CONSTITUENT in the TDB module.