TCS Al-alloys Mobility Database (MOBAL8)

Technical Information

Available Starting with Thermo-Calc Version 2024a

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Contents

MOBAL8: TCS Al-alloys Mobility Database

The TCS Al-alloys Mobility Database MOBAL8 is a kinetic database containing atomic mobility data for Al-based alloys. It provides kinetic data for those working with the add-on kinetic modules—the Diffusion Module (DICTRA) and the Precipitation Module (TC-PRISMA)—as well as a few specific calculation types, such as Scheil with back diffusion.

MOBAL8 is compatible and recommended for use in combination with TCAL9, TCS thermodynamic database of Al-based Alloys.

With the Diffusion Module (DICTRA), MOBAL8 can be used to study several different phenomena of interest to aluminum alloys, such as e.g. microsegregation during solidification, homogenization kinetics, growth/dissolution kinetics of precipitates, and much more. In a similar way, it is also suitable for simulating concurrent nucleation, growth, and coarsening of precipitates in Al alloys by using the Precipitation Module (TC-PRISMA).

MOBAL: TCS Aluminum Mobility Database Revision History. The current version of the database is MOBAL8.

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 for some databases, important higher order systems. This enables predictions to be made for multicomponent systems and alloys of industrial importance. Among these, the thermodynamic database is of fundamental importance.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

Additional Resources

Go to the Aluminum-based Alloys Databases page on our website where you can the technical information plus learn more about the compatible thermodynamic database. Also explore further applications of Thermo-Calc to aluminum including links to resources such as publications, webinars, videos, and more.

MOBAL8 Elements and Phases

Included Elements

There are 48 elements included in the most recent version of the database.

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

Included Phases

FCC_A1	FCC_L12	LIQUID

The phases have diffusion data included in the database. You can include other phases in a diffusion simulation. However, these other phases are treated as so-called diffusion NONE, i.e. there is no diffusion considered in these other phases. Any phase not listed above is automatically entered as diffusion NONE (in Console Mode in the DICTRA module or in Graphical Mode with the Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA)), as long as a thermodynamic description for the phases is retrieved prior to reading data from the mobility database.

Limits

The database is applicable for most commercial Al-based alloys, and care should be taken with alloys including high amounts of alloying elements.

As in the spirit of the CALPHAD method, predictions can be made for multicomponent systems by extrapolation into multicomponent space of data critically evaluated and assessed based on binary, ternary and in some cases higher order systems. However, critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software AB is interested to know about any significant deviations in order to improve any future release.

MOBAL8 Assessed Systems

This database contains critically assessed self- and impurity-diffusion data for the elements in the LIQUID, FCC_A1, and FCC_L12 phases on the basis of experimental information and empirical rules.

Complete and critical assessments of the important binary, ternary, and quaternary systems for the LIQUID, FCC_A1, and FCC_L12 phases are also included. Diffusion data for the LIQUID phase is assessed for systems where experimental data is available; otherwise the modified Sutherland equation is used for estimation.

FCC_L12 is modeled with the so-called partitioning model and has an energy contribution from a disordered A1-type solution, which is similar to the FCC_A1 phase.

Not all L12-type compounds are modeled as the FCC_L12 phase. Check if diffusion data are available for the phases and the systems that are (to be) involved in calculations.

Binary Systems

FCC_A1

FCC_A1 Assessed Binary Systems				
Ag-Al	Ag-Cu	Ag-Zn	Al-Cu	Al-Li
Al-Mg	Al-Ni	Al-Si	Cu-Fe	Cu-Mg
Cu-Mn	Cu-Ni	Cu-Si	Cu-Sn	Cu-Zn
Fe-Mn	Fe-Ni	Fe-Zn	Mn-Ni	Mo-Ni
Ni-Si	Ni-Zn			

LIQUID

Mobility parameters for self- and impurity- diffusivity of elements in all binary systems are assessed based on the experimental data available, or estimated by using the Modified Sutherland equation.

Ternary Systems

FCC_A1

FCC_A1 Assessed Ternary Systems			
Al-Ag-Cu	Al-Ag-Zn	Al-Cu-Fe	Al-Cu-Mg
Al-Cu-Mn	Al-Cu-Ni	Al-Cu-Si	Al-Cu-Sn
Al-Cu-Zn	Al-Fe-Ni	Al-Mg-Si	Al-Mg-Zn
Al-Mn-Ni	Cu-Fe-Ni	Cu-Fe-Mn	Cu-Mn-Ni
Cu-Mn-Zn	Cu-Ni-Si	Cu-Ni-Zn	

MOBAL: TCS Aluminum Mobility Database Revision History

Current Database Version

Database name (acronym):	**TCS Al-alloys Mobility Database (MOBAL)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**8.0**
First release:	**MOBAL1 was released in 2010**

MOBAL1 continues to be compatible with the TT Al-based Alloys Database (TTAL8). However, all other subsequent versions of this database (i.e. MOBAL2 and newer) are intended for use with the TCS Al-based Alloy Database (TCAL) database.

Changes in the Most Recent Database Release

MOBAL7.0 to MOBAL8.0

Software release 2024a (December 2023/January 2024)

- New Elements: Ba, Sb, Ta, and W
- Assessments for FCC_A1 Phase
  - New assessments for Ag-Cu, Ag-Zn, Al-Li, Al-Ag-Cu, Al-Ag-Zn, Al-Cu-Sn
  - Improved for Al-Si
  - Added mobility of impurity diffusivity for Al-Ba, Al-Sb, Al-Ta, and Al-W
- Assessments for Liquid Phase
  - Mobility parameters for self- and impurity- diffusivity of the systems not previously included in MOBAL version 7 and earlier are estimated using the Modified Sutherland equation.

Previous Releases

MOBAL6.0 to MOBAL7.0

Software release 2022a (December 2021/January 2022)

- Addition of five elements Nd, Pr, S, Se, and Te in the FCC and liquid phases.
- The atomic mobility data of Hf in the fcc phase was updated.
- A typo error that leads to wrong interaction between Si and Sn in the fcc phase was corrected.

MOBAL5.0 to MOBAL6.0

Software release 2021a (December 2020/January 2021).

- Three elements added to the database: Nb, P, and Y.

MOBAL4.0 to MOBAL5.0

Software release 2019a (December 2018).

- Added Mo and Al-Mo.
- 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.

MOBAL3.0 to MOBAL4.0

Software release version: 2018a (April 2018)

The main changes to the TCS Aluminum-alloys Mobility Database (MOBAL4) compared with MOBAL3 are that it:

- Contains a new element Er
- Has an improved description of liquid
- Has many updated and new binaries and now includes ternary and quaternary descriptions:
    - 3 phases
    - 37 binary systems
    - 20 ternary systems
    - 2 quaternary systems

MOBAL2.0 to MOBAL3.0

Software release version: 3.1 (December 2013)

- Mobility data for the new elements Be, Bi, Cd, Ce, Co, Ga, In and Pb in TCAL2 have been added for FCC_A1 and LIQUID phases.
- The mobility data for the interstitial elements B, C and H in the ordered phase FCC_L12 are now accessible thanks to the modified treatment of interstitials in ordered phases in DICTRA.
- The description of diffusion in the LIQUID phase has been greatly improved.