

TCS Al-alloys Mobility Database (MOBAL6)

Technical Information

Available Starting with Thermo-Calc Version 2021a



Contents

TCS Al-alloys Mobility Database (MOBAL6)	1
MOBAL6: TCS Al-alloys Mobility Database	3
Included Elements (39)	3
Included Phases	3
Assessed Systems	3
Limits	4
Additional Resources	4
MOBAL: TCS Aluminum Mobility Database Revision History	5

MOBAL6: TCS Al-alloys Mobility Database

The TCS Al-alloys Mobility Database MOBAL6 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.

MOBAL6 is compatible and recommended for use in combination with TCAL7, TCS thermodynamic database of Al-based Alloys.

With the Diffusion Module (DICTRA), MOBAL6 can be used to study several different phenomena of interest to aluminium 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).

Included Elements (39)

Ag	Al	В	Ве	Bi	С	Ca	Cd	Ce	Со
Cr	Cu	Er	Fe	Ga	Ge	Н	Hf	In	К
La	Li	Mg	Mn	Мо	Na	Nb	Ni	Р	Pb
Sc	Si	Sn	Sr	Ti	V	Υ	Zn	Zr	

Included Phases

FCC A1, FCC L12, and LIQUID



The above 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.

Assessed Systems

MOBAL6 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.

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.

Additional Resources

This document is available on our website on the <u>Aluminum-based Alloys Databases</u> page, where you can also learn more about the compatible thermodynamic database. Alternatively, when in Thermo-Calc, press F1 to search the online help for more information.

Also see our website for further <u>applications of Thermo-Calc to aluminum</u> including links to other resources such as publications, examples, and background information about the <u>CALPHAD methodology</u> used during the database development, plus much more.



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: 6.0



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

MOBAL5.0 to MOBAL6.0

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

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

Previous Releases

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 Aluminium-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.