TCS Steels/Fe-Alloys Mobility Database (MOBFE6)

Technical Information

Available Starting with Thermo-Calc Version 2021a

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Contents

MOBFE6: TCS Steels/Fe-Alloys Mobility Database

The TCS Steels/Fe-Alloys Mobility Database MOBFE6 is a kinetic database containing mobility data limited to Fe-based alloys. Data is present in a format suitable for simulation of diffusion controlled phenomena using the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA), and/or for use together with any Thermo-Calc programming interface.

MOBFE6 is compatible and recommended for use in combination with the TCFE11 (TCS Steels/Fe-Alloys Database) thermodynamic database.

Primarily for aiding alloy design and the optimization of manufacturing processes, through simulation of different diffusion controlled phenomena, such as e.g. microsegregation during solidification, homogenization, kinetics of phase transformations, precipitate growth/dissolution kinetics, carburization, nitriding, and much more.

Included Elements (28)

Al	B	C	Ca	Ce	Co	Cr	Cu	Fe	H
Mg	Mn	Mo	N	Nb	Ni	O	P	Ru	S
Si	Ta	Ti	W	V	Y	Zn	Zr		

Included Phases

BCC_A2	CEMENTITE	FCC_A1	FE4N_LP1	HCP_A3	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.

A model from Jönsson includes the effect on diffusion from the ferromagnetic transition in body-centred cubic Fe [B. Jönsson, “On Ferromagnetic Ordering and Lattice Diffusion: A Simple Model,” Zeitschrift für Met., vol. 83, pp. 349–355, 1992]. Diffusion data for the LIQUID phase has been assessed for systems where experimental data is available; otherwise the modified Sutherland equation was used for estimation. For the phase HCP_A3 most data are assumed to be the same as that in FCC_A1.

Assessed Systems

This database contains assessed self- and impurity diffusion data for a number of elements, as well as assessed data for some alloy systems (listed below). Since a lot of experimental data is missing in the literature, naturally some parameters are missing in the database. In order to make the database as complete as possible, some parameters have been estimated.

Binary Systems

BCC_A2

Al-Fe	B-Fe	C-Fe	C-Cr	Cr-Fe
Cr-H	Cr-N	Cr-Ni	Fe-H	Fe-N
Fe-Mo	Fe-Ni	Fe-O	Mo-H	Nb-H
Ti-H	Ta-H	V-H		

FCC_A1

Al-Cr	Al-H	Al-Ni	B-Fe	C-Co
C-Fe	C-Ni	Co-Fe	Co-H	Co-Ni
Co-W	Cr-Fe	Cr-Ni	Cu-Fe	Cu-H
Fe-H	Fe-Mn	Fe-N	Fe-Ni	Fe-O
Fe-Ru	Fe-Si	Fe-Zn	H-Ni	Mn-Ni

HCP_A3

Al-H	C-Fe	Co-H	Fe-N	Ti-H

FE4N

C-Fe	Fe-N			

LIQUID

Al-Ce	Al-Cu	Al-H	Al-Mg	Al-Ni
Al-Si	Al-Zn	Ce-Ni	Cu-H	Fe-H

Fe-Mn	Fe-Si	H-Ni	H-Si	Mg-H
Mg-Zn	Ni-Si			

Ternary Systems

BCC_A2

C-Cr-Fe	C-Fe-Mn	Fe-Cr-Mo	Fe-H-Si	Fe-Mn-Si
Fe-Mo-Mn	Cr-Fe-H	H-Mo-Ti	H-Nb-V	H-Ti-V

FCC_A1

Al-Cr-Ni	C-Cr-Fe	C-Fe-Mn	C-Fe-Ni	Co-Fe-Ni
Co-H-Ni	Cr-Fe-H	Cu-Fe-Mn	Fe-H-Ni	Fe-Mn-Si
Fe-Mo-Mn				

LIQUID

Co-Fe-H	Cr-Fe-H	Cu-Fe-H	Fe-H-Mn	Fe-H-Mo
Fe-H-Ni	Fe-H-Nb	Fe-H-V	Fe-H-W	

Higher Order Systems

BCC_A2

C-Cr-Fe-N-Ni

FCC_A1

C-Cr-Fe-Ni

Limits

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 Steel and Fe-Alloys Databases page, where you can also learn more about the compatible thermodynamic database.

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

MOBFE: TCS Steel and Fe- Mobility Database Revision History

Current Database Version

Database name (acronym):	**TCS Steels/Fe-Alloys Mobility Database (MOBFE)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**6.0**
First release:	**MOBFE1 was released in 2009**

Changes in the Most Recent Database Release

MOBFE5 to MOBFE6

Software release version: 2021a (December 2020/January 2021)

Addition of Hydrogen (H) to the database with the following assessed systems:

- FCC_A1: Al-H, Co-H, Cu-H, Fe-H, H-Ni, Fe-H-Ni, Cr-Fe-H, Co-H-Ni
- BCC_A2: Cr-H, Fe-H, Mo-H, Nb-H, Ti-H, Ta-H, V-H, Fe-H-Si, Cr-Fe-H, H-Mo-Ti, H-Nb-V, H-Ti-V
- HCP_A3: Al-H, Co-H, Ti-H
- LIQUID: Al-H, Cu-H, Fe-H, Mg-H, H-Ni, H-Si, Co-Fe-H, Cr-Fe-H, Cu-Fe-H, Fe-H-Mn, Fe-H-Mo, Fe-H-Ni, Fe-H-Nb, Fe-H-V, Fe-H-W

Previous Releases

MOBFE4 to MOBFE5

Software release version: 2020a (January 2020)

- Added new element Ru and mobility of Ru.
- Added mobility of C and W in FCC-Co.
- Revised default composition sets (type_defs).
- Updated the reference states of elements according to PURE5.

MOBFE3 to MOBFE4

Software release version: 2017a (March 2017)

Ce has been added in MOBFE4. The self-diffusion and impurity diffusion data related to Ce were included in the BCC_A2, FCC_A1, HCP_A3 and LIQUID phases. Mobility data for several Mn containing binary and ternary systems was also added. Diffusion data for the LIQUID phase has also been assessed for systems where experimental data is available; otherwise the modified Sutherland equation was used for estimation. Therefore, the description of the LIQUID phase has been entirely updated in this version of the database, from a constant value (1·10-9 [m/s2]) to temperature dependent ones. In addition to pure element data, complete and critical assessments for the LIQUID phase in 11 binary systems are implemented.

MOBFE2 to MOBFE3

Software release version: 2015a (June 2015)

The change from MOBFE2 to MOBFE3 is the addition of atomic mobilities of Y and Zn in bcc, fcc and liquid Fe.