TCS Ni-alloys Mobility Database (MOBNI6)

Technical Information

Available Starting with Thermo-Calc Version 2022b

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Contents

MOBNI6: TCS Ni-alloys Mobility Database

The TCS Ni-alloys Mobility Database (MOBNI) is a kinetic database containing mobility data for Ni-based alloys presented in a format suitable for simulation of diffusion controlled phenomena using the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA) as well as a few specific calculation types, such as Scheil with back diffusion.

MOBNI6 is compatible and primarily recommended for use in combination with the TCNI12 TCS Ni-based Superalloys thermodynamic database.

MOBNI: TCS Nickel Mobility Database Revision History. The current version of the database is MOBNI6.

Included Elements

There are 29 elements included in the most recent version of the database.

Al	B	C	Ca	Co	Cr	Cu	Fe	Hf	Mg
Mn	Mo	N	Nb	Ni	O	P	Pd	Pt	Re
Ru	S	Si	Ta	Ti	V	W	Y	Zr	

Included Phases

FCC_A1 (γ)	FCC_L12 (γ′)	BCC_A2 (α)
BCC_B2 (β)	LIQUID	IONIC_LIQ

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.

Assessed Systems

FCC_A1

The database contains assessed impurity diffusion data in Ni for all included elements. It also includes complete and critical assessments for FCC_A1 in the following binary and ternary systems.

Binary

FCC_A1 Binary Assessed Systems									
Al-B	Al-Cr	Al-Fe	Al-Ni	Al-Pt	Al-Ru	B-Ni	C-Cr	C-Fe	C-Ni
Co-Fe	Co-Mn	Co-Ni	Co-Pd	Co-Pt	Co-Re	Cr-Fe	Cr-Ni	Cu-Mn	Cu-Ni
Cu-Si	Fe-Ni	Fe-Pd	Fe-Pt	Hf-Ni	Mo-Ni	Mn-Ni	Nb-Ni	Ni-O	Ni-Pd
Ni-Pt	Ni-Re	Ni-Ru	Ni-Si	Ni-Ta	Ni-Ti	Ni-V	Ni-W	Ni-Y	Ni-Zr

Ternary

FCC_A1 Ternary Assessed Systems							
Al-B-Ni	Al-Cr-Ni	Al-Mn-Ni	Al-Ni-Pt	Al-Ni-Ti	C-Cr-Fe	C-Cr-Ni	C-Fe-Ni
Co-Cr-Mo	Co-Cr-W	Co-Fe-Ni	Co-Mo-W	Co-Ti-V	Co-V-W	Cr-Fe-Ni	Cu-Mn-Ni
Cu-Ni-Si	Ni-Al-Co	Ni-Al-Nb	Ni-Al-Ta	Ni-Al-W	Ni-Co-Cr	Ni-Co-Mo	Ni-Co-Re
Ni-Co-Ru	Ni-Co-W	Ni-Cr-Mo	Ni-Cr-Nb	Ni-Cr-Pt	Ni-Cr-V	Ni-Cu-Cr	Ni-Cu-Mo
Ni-Cu-Ti	Ni-Fe-Ti	Ni-Fe-V	Ni-Mo-Ta	Ni-Mo-W	Ni-Ti-Cr		

Quaternary

FCC_A1 Quaternary Assessed System
C-Cr-Fe-Ni

FCC_L12

Besides the Al-Ni system itself, the diffusion of the elements listed below in Ni_3Al have been optimized and validated against experimental data. For the remaining elements some estimates based on judgment are made.

FCC_L12									
B	Co	Cr	Fe	Hf	Mn	Mo	Nb	Pd	Pt
Re	Ru	Si	Ta	Ti	V	W			

BCC_A2

This phase does normally not appear in Ni-base superalloys, at least not in any larger quantities. Even so, there is a need for a description of this phase in order to successfully model the mobilities in the ordered bcc phase. The description for this phase is based on the description available in the MOBFE database.

BCC_B2

For this phase several of the binary systems in which this phase is present are optimized, e.g.

Al-Co	Al-Fe	Al-Ni	Co-Fe	Co-Ti	Ni-Ti

In addition, the diffusion of the following third elements in NiAl was studied and assessed. For the remaining elements some estimates based on judgment are made.

Co	Cr	Fe	Mo	Nb	Pd	Pt	Ta	Ti	V	W

LIQUID

The description for the liquid is based on an assessment of the ternary Al-Fe-Ni system. In addition diffusivities for Mo, Re and W diffusion in Ni are optimized. The diffusivities of Ca, Mg and S are estimated using the modified Sutherland equation, whereas remaining elements due to lack of consistent data is expected to diffuse like 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

Go to the Nickel-based Superalloys Databases page on our website where you can access technical information plus learn more about the compatible thermodynamic database. Also explore further applications of Thermo-Calc to nickel including links to resources such as examples, publications, and more.

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

MOBNI: TCS Nickel Mobility Database Revision History

Current Database Version

Database name (acronym):	**TCS Ni-alloys Mobility Database (MOBNI)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**6.0**

MOBNI version 2 and above (i.e. MOBNI2, MOBNI3, MOBNI4 and so forth) is the specialized nickel-based superalloys database and is intended for use with the TCS Ni-based Superalloys Database (TCNI) database. MOBNI1 is compatible with the TTNI8 database.

Changes in the Most Recent Database Release

MOBNI5.1 to MOBNI6

Software release version: 2022b (June 2022)

New Element

- Phosphorus (P) is added to make it a 29 element framework.

FCC_A1 Phase

Mobility parameters for 29 binary or ternary systems are added or reassessed:

- Four (4) binaries: Co-Mn, Co-Re, Cr-Pt and Ni-P
- Twenty-five (25) ternaries: Co-Cr-Mo, Co-Cr-W, Co-Mo-W, Co-Ti-V, Co-V-W, Ni-Al-Co, Ni-Al-Nb, Ni-Al-Ta, Ni-Al-W, Ni-Co-Cr, Ni-Co-Mo, Ni-Co-Re, Ni-Co-Ru, Ni-Co-W, Ni-Cr-Mo, Ni-Cr-Nb, Ni-Cr-Ti, Ni-Cr-V, Ni-Cu-Cr, Ni-Cu-Mo, Ni-Cu-Ti, Ni-Fe-Ti, Ni-Fe-V, Ni-Mo-Ta, and Ni-Mo-W

FCC_L12 Phase

- Mobility parameters for three (3) ternary systems are added or reassessed: Ni-Al-Ta, Ni-Al-Re, and Ni-Al-W.

BCC_B2 Phase

- Mobility parameters for one ternary system are assessed: Ni-Al-Co.

LIQUID Phase

- Mobility parameters for one binary system are added: Ni-P

Previous Releases

MOBNI5 to MOBNI5.1

Software release version: 2020a (January 2020).

- Revised default composition sets (type_defs).
- Updated the reference states of elements according to PURE5

MOBNI4 to MOBNI5

Software release version: 2019a (January 2019).

The change from MOBNI4 to MOBNI5 is the addition of atomic mobilities of Ca, Mg, and S in FCC_A1, L12, BCC_A2, B2 and liquid phases.

MOBNI3 to MOBNI4

Software release version: 2015a (June 2015). Compatible with the TCNI database.

The change from MOBNI3 to MOBNI4 is the addition of atomic mobilities of Cu in fcc, L12, B2 and liquid phases.

MOBNI2 to MOBNI3

Software release version: 4.0 (June 2014). Some updates with 4.1 (November 2014). Compatible with the TCNI database.

The descriptions for interstitial elements B, C, and N are now included.

The description of the liquid using the ionic liquid model and MQ parameters is now available and compatible with TCNI7.

The parameters have been updated for the following systems:

- For the FCC phase: Ni-Mo, Ni-O, Ni-Ru, Ni-Si, Ni-Ti, Ni-V, Ni-Y, Al-Pt, Al-Ru and Ni-Al-Pt.
- For the L12 phase: Ni-Fe, Ni-Al-Mo, Ni-Al-Pt, Ni-Al-Ru, Ni-Al-Re and Ni-AlV.

The following systems have been checked against new assessments or experimental data:

- For the FCC phase: Ni-Hf, Ni-Nb, Ni-Pt, Ni-Re, Ni-Zr, Ni-Al-W, Ni-Al-Re, NiAl-Ru, Ni-Co-Re, Ni-Co-Ru, Ni-Re-Ru and Ni-Ru-W.
- For the L12 phase: Ni-Al-Fe, Ni-Al-Si and Ni-Al-Ti
- For the B2 phase: Ni-Al-Ru

MOBNI2 to MOBNI3

Software release version: 4.1 (November 2014). Compatible with the TCNI database.

- The mobility of Mn has been added. This means that MOBNI3 is in complete alignment with TCNI7.
- The mobility data for the liquid phase have been adapted to the corresponding new thermodynamic descriptions in TCNI7.
- Various minor corrections and adjustments have been implemented.