TCS Ni-alloys Mobility Database (MOBNI7)

Technical Information

Available Starting with Thermo-Calc Version 2026b

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Contents

MOBNI7: 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.

MOBNI7 is compatible and primarily recommended for use in combination with the TCNI14 TCS Ni-based Superalloys thermodynamic database.

MOBNI: TCS Nickel Mobility Database Revision History. The current version of the database is MOBNI7.

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. Also visit the video tutorials on our website or our YouTube playlist.

Learn More

Go to the Nickel-based Superalloys Databases page on our website where you can access this *Technical Information* plus learn more about the compatible thermodynamic database and its *Validation and Calculation Examples Collection*. Also explore further applications of Thermo-Calc to nickel including links to resources such as examples, publications, and more.

MOBNI7: Elements and Phases

Included Elements

There are 30 elements included in the most recent version of the database.

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

Included Phases

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.

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.

MOBNI7: Assessed Binary 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 systems.

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

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 Binary Assessed Systems									
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.

BCC_B2 Binary Assessed Systems										
Al-Co	Al-Fe	Al-Ni	Co-Cr	Co-Fe	Co-Ti	Cr-Fe	Cr-Ni	Fe-Ni	Fe-Si	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.

BCC_B2 Estimates										
Co	Cr	Fe	Mo	Nb	Pd	Pt	Ta	Ti	V	W

MOBNI7: Assessed Ternary 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 ternary systems.

FCC_A1 Ternary Assessed Systems							
Al-B-Ni	Al-Co-Ni	Al-Cr-Ni	Al-Mn-Ni	Al-Nb-Ni	Al-Ni-Pt	Al-Ni-Ta	Al-Ni-Ti
Al-Ni-W	C-Cr-Fe	C-Cr-Ni	C-Fe-Ni	Co-Cr-Mo	Co-Cr-Ni	Co-Cr-W	Co-Fe-Ni
Co-H-Ni	Co-Mo-Ni	Co-Mo-W	Co-Ni-Re	Co-Ni-Ru	Co-Ni-W	Co-Ti-V	Co-V-W
Cr-Cu-Ni	Cr-Fe-H	Cr-Fe-Ni	Cr-Mo-Ni	Cr-Nb-Ni	Cr-Ni-Pt	Cr-Ni-Ti	Cr-Ni-V
Cu-Mn-Ni	Cu-Mo-Ni	Cu-Ni-Si	Cu-Ni-Ti	Fe-H-Ni	Fe-Ni-Ti	Fe-Ni-V	Mo-Ni-Ta
Mo-Ni-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 self-diffusivity and impurity- diffusivity of the remaining elements are estimated using the Modified Sutherland equation.

MOBNI7: Assessed Quaternary Systems

FCC_A1

FCC_A1 Quaternary Assessed System
C-Cr-Fe-Ni

MOBNI7: Models for the Included Phases

Phase Name	Prototype	Strukturbericht	Pearson Symbol	Space Group	Info	Sublattices	Formula Unit
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)	-	2	(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, S, SI, TA, TI, V, W, Y, ZR)1(B, C, H, N, O, VA)1
DIS_FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	(225, Fm-3m)	-	2	(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, S, SI, TA, TI, V, W, Y, ZR)1(B, C, H, N, O, VA)1
FCC_L12	Bogdanovite (Cu3Au, L12)	L12	cP4	(221, Pm-3m)	-	3	(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, S, , SI, TA, TI, V, W, Y, ZR)0.75 (AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, S, , SI, TA, TI, V, W, Y, ZR)0.25(B, C, H, N, O, VA)1
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	(229, Im-3m)	-	2	(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, S, , SI, TA, TI, V, W, Y, ZR, VA)1 (B, C, H, N, O, VA)3
BCC_B2	CsCl (B2)	B2	cP2	(221, Pm-3m)	-	3	(AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, , S, SI, TA, TI, V, W, Y, ZR, VA)0.5 (AL, CA, CO, CR, CU, FE, HF, MG, MN, MO, NB, NI, P, PD, PT, RE, RU, , S, SI, TA, TI, V, W, Y, ZR, VA)0.5 (B, C, H, N, O, VA)3
LIQUID	Liquid	-	-	-	LIQUID mixture.	1	(AL, AL1N1, AL2/3O1, AL2/3S, AL4/3O2, B, BO3/2, C, CA, CAO, CAS, CO, COO, COO3/2, COS, CR, CRO, CRO3/2, CRS, CU, CU2O, CU2S1, CUO, FE, FEO, FEO3/2, FES, H, HF, HF1/2O1, MG, MGO, MGS, MN, MNO, MNO3/2, MNS, MO, MO1/2O1, MO1/2S, MOO3, N, NB, NB1O1, NBO2, NBO5/2, NBS, NI, NIO, NIS, P, P2/5S1, PD, PDO, PT, PTO, RE, RE1/2O1, REO7/2, RU, RU1/2O1, RU1/2S1, S, SI, SI1/2O1, SI1/2S, SIO2, SI2O4, TA, TA2/5O1, TI, TIO, TIO2, TIS, V, VO, VO2, VO5/2, VS, W, W1/3O1, W1/3S1, Y, Y2/3O1, ZR, ZR1/2O1, ZR1/2S1)1

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:	7.0
First release:	MOBNI1 was released in 2000-2001

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.

MOBNI6.1 to MOBNI7.0

Software release version: 2026b (June 2026)

Elements

Added 1 new element: H (30 elements total).

Binary Systems

The following binary systems for the FCC_A1 phase are newly added or re-assessed:

- New: Co-Ti
- Reassessed: Co-Re, Co-V, Mo-Ni, Ni-Re, Ni-Ta, Ni-Ti, and Ni-W

Ternary Systems

The following ternary systems for the FCC_A1 phase are newly added or re-assessed:

- New: Co-H-Ni, Cr-Fe-H, and Fe-H-Ni
- Reassessed: Al-Ni-Ta, Al-Ni-W, Co-Cr-Ni, Co-Cr-W, Co-Mo-W, Co-Ni-Re, Co-Ni-W, Co-Ti-V, Cr-Mo-Ni, Cr-Ni-Ti, Mo-Ni-Ta, and Mo-Ni-W

MOBNI6.0 to MOBNI6.1

Software release version: 2025a (January 2025)

- Reassessment of FCC_L12 in Ni-Ta system.

MOBNI5.1 to MOBNI6.0

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

MOBNI5.0 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.

MOBNI3 to MOBNI3.1

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.

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