

TCS Ti-alloys Mobility Database (MOBTI5)

Technical Information

Available Starting with Thermo-Calc Version 2024b



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MOBTI5: TCS Ti-alloys Mobility Database

The TCS Ti-alloys Mobility Database (MOBTI) is a kinetic database containing atomic mobility data limited to Ti/TiAl-based alloys.

MOBTI5 is compatible and recommended for use in combination with the TCTI6 TCS Ti/TiAl-based Alloys thermodynamic database.

When the database is used with the Add-on Diffusion Module (DICTRA), you can study several diffusion-controlled phenomena in Ti/TiAl based alloys, such as microsegregation during solidification, homogenization kinetics, growth/dissolution kinetics of precipitates, and much more.

Similarly when combined with the Add-on Precipitation Module (TC-PRISMA), is suitable to simulate concurrent nucleation, growth, and coarsening of precipitates in Ti/TiAl-alloys.



[MOBTI: TCS Titanium Mobility Database Revision History](#). The current version is MOBTI5.

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 [Titanium and TiAl-based Alloys 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 titanium and TiAl](#) including links to resources such as examples, publications, and more.

MOBTI5: Elements and Phases

Included Elements

There are 28 elements included in the most recent version of the database.

Ag	Al	B	C	Co	Cr	Cu	Fe	H	Hf
Mn	Mo	N	Nb	Ni	O	Pd	Pt	Re	Ru
Si	Sn	Ta	Ti	V	W	Y	Zr		

Included Phases

Solution Phases

Solution Phases		
BCC_A2	HCP_A3	LIQUID

Compounds

Compunds	
Ti3Al (ALTI3_D019)	TiAl (ALTI_L10)



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.

MOBTI5: Assessed Systems

This version of TCS Ti-alloys Mobility Database (MOBTI) contains critically assessed self- and impurity diffusion data for the elements in the LIQUID, BCC_A2, HCP_A3, ALTi_L10, and ALTi3_D019 phases when experimental information is available. In other cases, estimates based on empirical rules are made.

This database also includes complete and critical assessments of the binary and ternary systems for the LIQUID, BCC_A2, HCP_A3, ALTi_L10, and ALTi3_D019 phases.

Diffusion data for the LIQUID phase is also assessed for systems where experimental data is available; otherwise the modified Sutherland equation is used for estimation.

- 46 binary and 28 ternary/quaternary- systems for solid solution phases, 14 elements in the ALTi_L10 compound, and six (6) elements in the ALTi3_D019 compound are assessed.
- Mobility parameters for self- and impurity- diffusivity of elements in all binary systems of LIQUID phase are assessed based on the experimental data available, or estimated by using the Modified Sutherland equation.

Binary Systems

BCC_A2

Binary Systems (BCC_A2)									
Ag-Ti	Al-Fe	Al-Nb	Al-Ni	Al-Sn	Al-Ti	Al-V	Cr-Mn	Cr-Nb	Cr-Ti
Cu-Ti	Fe-Ti	Fe-V	H-Mo	H-Nb	H-Ti	H-V	Hf-Ti	Mo-Nb	Mo-Ti
Nb-Ta	Nb-Ti	Nb-V	Nb-W	Ni-Ti	Si-Ti	Sn-Ti	Ta-Ti	Ti-Mn	Ti-Pd
Ti-V	Ti-W	Ti-Zr	Zr-Hf	Zr-Nb	Zr-Ta				

HCP_A3

Binary Systems (HCP_A3)				
Ag-Ti	Al-H	Cu-Ti	H-Ti	Pd-Ti

ALTI_L10

Binary Systems (ALTI_L10)

Al-Ti

ALTI3_D019

Binary Systems (ALTI3_D019)

Al-Ti

LIQUID

Binary Systems (LIQUID)

Al-Ni	Al-Si	Fe-Mn	Fe-Si	Ni-Si
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Ternary Systems

BCC_A2

Ternary Systems (BCC_A2)

H-Mo-Ti	H-Nb-V	H-Ti-V	Al-Cr-Ti
Al-Fe-Ti	Al-Mo-Ti	Al-Ti-V	Ti-Al-Zr
Ti-Al-Nb	Ti-Al-Sn	Ti-Cr-Mn	Ti-Nb-Ta
Ti-Nb-Zr	Zr-Ta-Nb	Ti-Cr-V	Ti-Mo-Nb
Ti-Fe-V	Ti-Fe-Nb	Ti-Cr-Zr	Ti-Nb-V
Ti-Al-Ni	Ti-Cr-Nb		

HCP_A3

Ternary Systems (HCP_A3)

H-Al-Ti

ALTI_L10

Ternary Systems (ALTI_L10)				
Al-Cr-Ti	Al-Mn-Ti	Al-Nb-Ti	Al-Ti-Zr	O-Al-Ti

ALTI3_D019

Ternary Systems (ALTI3_D019)				
H-Al-Ti	O-Al-Ti	Al-Ni-Ti	Al-Nb-Ti	

Quaternary Systems

BCC_A2

Quaternary Systems (BCC_A2)				
Ti-Nb-Zr-Hf	Ti-Nb-Zr-Ta	Ti-Nb-Zr-Cr	Ti-Nb-Zr-Sn	Ti-Nb-Zr-W

MOBTI: TCS Titanium Mobility Database Revision History

Current Database Version

Database name (acronym):	TCS Ti-alloys Mobility Database (MOBTI)
Database owner:	Thermo-Calc Software AB
Database version:	5.0
First release:	MOBTI1 was released in 2013



MOBTI versions 2 and higher are for use with the Thermo-Calc thermodynamic TCTI database. MOBTI1 is for use with the ThermoTech TTTI3 database.

Changes in the Most Recent Database Release

MOBTI4.1 to MOBTI5

Software release version: 2024b (June 2024)

New Phases

- New compound phase ALTI3_D019 is added, the corresponding mobility data for H, O, Al, Ni, Nb, and Ti elements are assessed, and the mobility data for other elements are estimated.

Updated Phases

- Four updated phases: BCC_A2, HCP_A3, LIQUID, and ALTI_L10.
- The description of diffusion in the LIQUID phase is greatly improved.
- Mobility data for the O element in the compound phase ALTI_L10 are added.

Updated Systems

- BCC_A2
 - Binary: Al-Nb, Al-Ni, Al-Sn, Cr-Mn, Cr-Nb, Fe-V, Mo-Nb, Nb-Ta, Nb-V, Nb-W, Ti-Mn, Ti-Pd, Ti-W, Zr-Hf, Zr-Nb, and Zr-Ta.
 - Ternary: Al-Mo-Ti, Ti-Al-Zr, Ti-Al-Nb, Ti-Al-Sn, Ti-Cr-Mn, Ti-Nb-Ta, Ti-Nb-Zr, Ti-Al-Ni, Ti-Cr-V, Ti-Mo-Nb, Ti-Fe-V, Ti-Fe-Nb, Ti-Cr-Zr, Ti-Cr-Nb, Ti-Nb-V, and Zr-Ta-Nb.
 - Quaternary: Ti-Nb-Zr-Hf, Ti-Nb-Zr-Ta, Ti-Nb-Zr-Cr, Ti-Nb-Zr-Sn, and Ti-Nb-Zr-W.

- HCP_A3
 - One binary system (Cu-Ti) for HCP_A3 phase is newly assessed.

Previous Releases

MOBTI4.0 to MOBTI4.1

Software release 2023a (December 2022/January 2023)

- Modified the impurity diffusivity parameter of nitrogen in HCP_A3 titanium.

MOBTI3.1 to MOBTI4.0

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

The element Copper (Cu) is added in the Bcc_A2, Hcp_A3, and liquid phases.

MOBTI3.0 to MOBTI3.1

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

The diffusivity of O in Bcc_A2 Ti is corrected.

MOBTI2.0 to MOBTI3.0

Software release version: 2019a (January 2019)

- 4 new elements added: Ag, H, Pd, Pt
- 7 new binary systems added: Ag-Ti, Al-H, H-Ti, H-V, H-Nb, H-Mo, Pd-Ti
- 4 new ternary systems added: H-Mo-Ti, H-Ti-V, H-Nb-V, H-Al-Ti

MOBTI1.0 to MOBTI2.0

Software release version: 2017a (June 2017)

The following is what is included with MOBTI2.

- 23 elements Al, B, C, Co, Cr, Fe, Hf, Mn, Mo, N, Nb, Ni, O, Re, Ru, Si, Sn, Ta, Ti, V, W, Y, Zr.
 - 4 phases: BCC_A2, HCP_A3, ALTI_L10, LIQUID.
 - 20 assessed binary systems.
 - 7 assessed ternary systems.
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