TCS Nb-based Alloys Mobility Database (MOBNB1)

Technical Information

Available Starting with Thermo-Calc Version 2024b

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MOBNB1: TCS Nb-based Alloys Mobility Database

Niobium-based alloys find applications in various industries due to their unique properties. They are commonly used in aerospace and aviation industries for manufacturing superalloys, which are heat-resistant and can withstand high-stress environments, such as jet engines and gas turbines. Niobium-based alloys are also used in medical implants due to their biocompatibility and corrosion resistance. Additionally, these are used in the production of superconductors for applications like MRI machines and particle accelerators. In the automotive sector, Nb-based alloys are used for lightweighting and improving the strength of structural components.

The TCS Nb-based Alloys Mobility Database (MOBNB) is a kinetic database containing atomic mobility data for Nb-based refractory alloys. The database is compatible and primarily recommended for use with the most recent version of the TCS Nb-based Alloys Database (TCNB) (i.e. TCNB1).

The Nb-based alloys thermodynamic and kinetic databases (i.e. TCNB1 and MOBNB1) are available for refractory alloys (Nb-based) that exhibit high melting temperature and low density compared to Ni-superalloys. Together the databases can be used to study the influence of alloying by the addition of elements on various properties.

The MOBNB1 database provides the kinetic data for those working with the Add-on Modules—the Diffusion Module (DICTRA) and the Precipitation Module (TC-PRISMA). It can also be used together with the Thermo-Calc Software Development Kits (SDKs).

When the kinetic database is used with the Diffusion Module (DICTRA), and a thermodynamic database for Nb-based alloys (e.g. TCNB1), you can study diffusion-controlled phenomena in Nb/substrate systems, such as solidification, growth of interfacial compounds, dissolution of substrates, interdiffusion, and much more. Similarly, when used with the Precipitation Module (TC-PRISMA) it is suitable to simulate concurrent nucleation, growth, and coarsening of precipitates in Nb alloys.

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 Niobium-based Alloys page on our website where you can access an examples collection and the technical information plus learn more about the compatible thermodynamic database.

MOBNB1 Elements and Phases

Included Elements

There are 12 elements included in the most recent version of the database.

Al	C	Cr	Hf	Mo	Nb
Si	Ta	Ti	V	W	Zr

Included Phases

Solution Phases

Solution Phases			
BCC_A2	FCC_A1	HCP_A3	LIQUID

Compound Phases

Compound Phases	
CRSI2_C40	NB5SI3_D8L

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.

MOBNB1 Assessed Systems

The following systems have been either critically or tentatively assessed.

- 32 binary systems
- 6 ternary systems
- 4 quaternary systems
- Nb and Si elements in 2 compounds

Mobility data for self- and impurity- diffusivity within the LIQUID phase are estimated using the Modified Sutherland equation. Mobility data for the other elements in the CRSI2_C40 and NB5SI3_D8L phases are also estimated.

Binary Systems

FCC_A1

Binary Systems (FCC_A1)	
Al-Si	C-Nb

BCC_A2

Binary Systems (BCC_A2)				
Al-Nb	Al-Ti	Al-V	Cr-Nb	Cr-Ta
Cr-Ti	Hf-Nb	Hf-Ta	Hf-Ti	Mo-Cr
Mo-Hf	Mo-Nb	Mo-Ta	Mo-Ti	Mo-W
Nb-Ta	Nb-Ti	Nb-V	Nb-W	Ta-Ti
Ta-W	Ti-V	Zr-Hf	Zr-Mo	Zr-Nb
Zr-Ta	Zr-Ti	Zr-V		

HCP_A3

Binary Systems (HCP_A3)	
C-Mo	C-Nb

Ternary Systems

BCC_A2

Ternary Systems (BCC_A2)					
Ti-Al-Nb	Ti-Cr-Nb	Ti-Nb-Ta	Ti-Nb-V	Zr-Ta-Nb	Zr-Ti-Nb

Quaternary Systems

BCC_A2

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

Compounds

Compounds	
CRSI2_C40: $NbSi_2$	NB5SI3_D8L: Nb_5Si_3