TCS High Entropy Alloy Mobility Database (MOBHEA3)

Technical Information

Available Starting with Thermo-Calc Version 2023a

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Contents

MOBHEA3: TCS High Entropy Alloy Mobility Database

The TCS High Entropy Alloy Mobility Database (MOBHEA) is a kinetic database containing atomic mobility data for high-entropy alloys (HEA) presented in a format suitable for simulation of diffusion controlled phenomena using the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA). It can also be used together with all Thermo-Calc programming interfaces.

In MOBHEA3, atomic mobilities for BCC_A2 phase are additionally assessed.

MOBHEA3 is compatible and primarily recommended for use in combination with the TCHEA6 thermodynamic database.

MOBHEA: TCS High Entropy Alloy Mobility Database Revision History. The current version of the database is MOBHEA3. See the link for any subversion release details.

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 High Entropy Alloys Databases page on our website where you can access an examples collection and the technical information plus learn more about the compatible kinetic database. Also explore further applications of Thermo-Calc to high entropy alloys including links to resources such as examples, publications, and more.

MOBHEA3 Elements and Phases

Included Elements

There are 26 elements included in the most recent version of the database.

Al	B	C	Co	Cr	Cu	Fe	Hf	Ir	Mn
Mo	N	Nb	Ni	Re	Rh	Ru	Si	Sn	Ta
Ti	V	W	Y	Zn	Zr				

Included Phases

FCC_A1	FCC_L12	BCC_A2	BCC_B2	LIQUID

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

The database is applicable for most Ti, V, Cr, Mn, Zr, Nb, Mo, Hf, Ta, W, Al, Fe-based alloys, and care should be taken with alloys including high amounts of alloying elements.

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.

MOBHEA3 Assessed Systems

The following systems have been either critically or tentatively assessed in this version of the database for BCC_A2 phase.

- 60 binary systems
- 25 ternary systems (21 critically assessed and 4 tentatively assessed)

Binary Systems

Assessed Binary Systems							
Al-Co	Al-Cr	Al-Fe	Al-Mn	Al-Mo	Al-Nb	Al-Ni	Al-Sn
Al-Ti	Al-V	Co-Cr	Co-Fe	Cr-Fe	Cr-Mn	Cr-Mo	Cr-Nb
Cr-Ni	Cr-Ta	Cr-Ti	Cr-V	Cu-Fe	Fe-Mn	Fe-Mo	Fe-Nb
Fe-Ni	Fe-Si	Fe-Ti	Fe-V	Fe-W	Fe-Zn	Hf-Mo	Hf-Ti
Hf-Zr	Mn-Si	Mn-Ti	Mn-V	Mn-Zr	Mo-Nb	Mo-Ni	Mo-Ta
Mo-Ti	Mo-W	Mo-Zr	Nb-Ni	Nb-Ta	Nb-Ti	Nb-V	Nb-W
Nb-Zr	Ni-Ti	Ni-V	Ni-W	Sn-Ti	Sn-V	Ta-Ti	Ta-W
Ta-Zr	Ti-V	Ti-Zr	V-Zr				

Ternary Systems

Critically Assessed Ternaries					
Al-Fe-Ni	Fe-Al-Mn	Fe-Al-Ti	Fe-Cr-Ni	Fe-Cr-V	Fe-Mn-Si
Fe-Mo-Cr	Ti-Al-Cr	Ti-Al-Mn	Ti-Al-Mo	Ti-Al-Nb	Ti-Al-Ni
Ti-Al-Sn	Ti-Al-V	Ti-Al-Zr	Ti-Cr-Mn	Ti-Cr-V	Ti-Mo-Zr
Ti-Ta-Nb	Zr-Ta-Nb	Zr-Ti-Nb			

Tentatively Assessed Ternaries			
Al-Mn-V	Al-Fe-V	Ti-Nb-Hf	Zr-Ta-Ti

MOBHEA: TCS High Entropy Alloy Mobility Database Revision History

Current Database Version

Database name (acronym):	**TCS High Entropy Alloy Mobility Database (MOBHEA)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**3.0**
First release:	**MOBHEA1 was released in 2018**

Changes in the Most Recent Database Release

MOBHEA2 to MOBHEA3

Software release 2023a (January 2023)

- Atomic mobility parameters for all BCC_A2 binary systems have been assessed or estimated and then updated.
- The database was validated in the Fe-Ti, Zr-Nb-Ta-Ti, Zr-Nb-Hf-Ti and Al-Fe-Cr-Mn-V systems.

Previous Releases

MOBHEA1 to MOBHEA2

Software release version: 2020a (January 2020)

- All atomic mobilities for pure elements have been updated.
- The CoCrFeNi, CoFeMnNi, and CoCrMnNi systems were assessed.
- The CoCrFeMnNi, CoCrCuFeNi, and AlCoCrFeNi systems were assessed.
- The database was validated in the AlCoCrFeNiTi system.
- Ir, Rh, Sn, and Zn have been added (26 element framework).