TCS High Entropy Alloy Mobility Database (MOBHEA2)

Technical Information

Available Starting with Thermo-Calc Version 2020a

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MOBHEA2: 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.

MOBHEA2 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 MOBHEA2. See the link for any subversion release details.

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.

Assessed Systems

The MOBHEA2 database is based on MOBNI4, and all relevant binary and ternary descriptions from MOBNI4 have been adopted directly. Furthermore, by considering all available HEA diffusivity measurements to date (2018-01-31), the atomic mobilities for the FCC_A1 phase in the HEA systems containing Al, Co, Cr, Cu, Fe, Mn, and Ni have been critically assessed. The resulting new atomic mobility parameters have been included in MOBHEA2. A systematic validation has been conducted for this mobility

database and it was found that a majority of experimental diffusion couple composition profiles could be satisfactorily simulated with the Diffusion Module (DICTRA) in Thermo-Calc by using MOBHEA2 and TCHEA6.

Limits

The database is applicable for most commercial Al-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.

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.

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

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:	**2.0**
First release:	**MOBHEA1 was released in 2018**

Changes in the Most Recent Database Release

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).