MOBHEA1: TCS High Entropy Alloy Mobility Database

Database name:	TCS High Entropy Alloy Mobility Database	*Database acronym:*	MOBHEA
Database owner:	Thermo-Calc Software AB	*Database version:*	1.0

MOBHEA1 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.

MOBHEA1 is compatible and primarily recommended for use in combination with the TCHEA3 thermodynamic database.

Included Elements (23)

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

Included Phases

FCC_A1 FCC_L12 BCC_A2 BCC_B2 LIQUID

Apart from the above phases for which diffusion data are included in the database, then also other phases may be included in a simulation. However, these other phases will be treated as so-called diffusion “NONE”, i.e. there will be no diffusion considered in such phases. Phases which are not listed above will automatically be entered as diffusion “NONE” in the DICTRA module in Thermo-Calc, provided a thermodynamic description for such phases has been retrieved prior to reading data from the mobility database.

Assessed Systems

The MOBHEA1 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 MOBHEA1. 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 MOBHEA1 and TCHEA3.

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 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.

Scientific Models and References

See the Thermo-Calc Software reference list and reference library at:
https://www.thermocalc.com/support/resources/