MOBHEA2: 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:*	2

MOBHEA2 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 TCHEA4 thermodynamic database.

Included Elements (26)

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 above 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 Calculator), 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 TCHEA4.

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.

Scientific Bibliography

See the Thermo-Calc Software scientific bibliography at: https://www.thermocalc.com/support/resources/.