MOBFE4: TCS Steels/Fe-Alloys Mobility Database

Database name:	TCS Steels/Fe-Alloys Mobility Database	*Database acronym:*	MOBFE
Database owner:	Thermo-Calc Software AB	*Database version:*	4.0

MOBFE is a kinetic database containing mobility data limited to Fe-based alloys. Data is present in a format suitable for simulation of diffusion controlled phenomena using the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA), and/or for use together with any Thermo-Calc programming interface. MOBFE is compatible and recommended for use in combination with the TCFE (TCS Steels/Fe-Alloys Database) thermodynamic database.

Applications

Primarily for aiding alloy design and the optimization of manufacturing processes, through simulation of different diffusion controlled phenomena, such as e.g. microsegregation during solidification, homogenisation, kinetics of phase transformations, precipitate growth/dissolution kinetics, carburization, nitriding and much more.

Included Elements (26)

Al	B	C	Ca	Ce	Co	Cr	Cu	Fe	Mg	Mn	Mo	N	Nb	Ni
O	P	S	Si	Ta	Ti	W	V	Y	Zn	Zr				

Included Phases

BCC_A2	CEMENTITE	FCC_A1	FE4N_LP1	HCP_A3	LIQUID

Please note that apart from the above phases for which diffusion data is indeed included in the database, other phases may be included in a diffusion 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

This database contains assessed self- and impurity diffusion data for a number of elements, as well as assessed data for some alloy systems (listed below). Since a lot of experimental data is missing in the literature, naturally some parameters are missing in the database. In order to make the database as complete as possible, some parameters have been estimated.

Binary systems

BCC_A2

Al-Fe	C-Fe	C-Cr	Cr-Fe	Cr-N	Cr-Ni	Fe-N	Fe-Mo	Fe-Ni

FCC_A1

Al-Cr	Al-Ni	C-Fe	C-Ni	Co-Fe	Co-Ni	Cr-Fe	Cr-Ni	Cu-Fe
Fe-Mn	Fe-N	Fe-Ni	Fe-Si	Mn-Ni				

HCP_A3

C-Fe	Fe-N

FE4N

C-Fe	Fe-N

LIQUID

Al-Ce	Al-Cu	Al-Mg	Al-Ni	Al-Si	Al-Zn	Ce-Ni	Fe-Mn	Fe-Si
Ni-Si	Mg-Zn							

Ternary systems

BCC_A2

C-Cr-Fe	C-Fe-Mn	Fe-Cr-Mo	Fe-Mn-Si	Fe-Mo-Mn

FCC_A1

C-Fe-Mn	Cu-Fe-Mn	Fe-Mo-Mn	Fe-Mn-Si
Al-Cr-Ni	C-Cr-Fe	C-Fe-Ni	Co-Fe-Ni

Higher order systems

BCC_A2

C-Cr-Fe-N-Ni

FCC_A1

C-Cr-Fe-Ni

A model from Jönsson includes the effect on diffusion from the ferromagnetic transition in body-centred cubic Fe (B. Jönsson; Z. Metallkd. 83(1992), pp 349-355). Diffusion data for the LIQUID phase has also been assessed for systems where experimental data is available; otherwise the modified Sutherland equation was used for estimation. For the phase HCP_A3 most data are assumed to be the same as that in FCC_A1.

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 in knowing 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: http://www.thermocalc.com/resources/