Thermo-Calc Software

Database name:TCS Alloy Mobility DatabaseDatabase owner:Thermo-Calc Software ABDatabase segment:Iron and Steel

Brief Description

MOB2 is a kinetic database containing mobility data primarily but not limited to Fe-based alloys. Data is present in a format suitable for simulation of diffusion controlled phenomena using the DICTRA simulation software, and/or for use together with any Thermo-Calc programming interface. MOB2 is compatible and recommended for use in combination with the SSOL (SGTE Solution Database) thermodynamic database, and also the TCFE5 (TCS Steels/Fe-Alloys Database version 5) and earlier versions of TCFE.

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

Ag	Al	Am	As	Au	В	Ва	Ве	Bi	С	Ca	Cd	Со	Cr	Cs	Cu	Dy
Er	Fe	Ga	Gd	Ge	Hf	Hg	Но	In	lr	К	La	Li	Lu	Mg	Mn	Мо
Ν	Na	Nb	Nd	Ni	Np	Os	Р	Ра	Pb	Pd	Pr	Pt	Pu	Rb	Re	Rh
Ru	S	Sb	Sc	Se	Si	Sm	Sn	Sr	Та	Tb	Тс	Те	Th	Ti	ΤI	Tm
U	V	W	Y	Yb	Zn	Zr										

Included Phases

BCC_A2CEMENTITEFCC_A1FE4NHCP_A3LIQUIDPlease note that apart from above phases for which diffusion data is indeed included in the database, then also other phasesmay be included in a DICTRA simulation. However, these other phases will be treated as so-called diffusion "NONE", i.e. therewill be no diffusion considered in such phases. Phases which are not listed above will automatically be entered as diffusion"NONE" in DICTRA, provided a thermodynamic description for such phases has been retrieved prior to reading data from themobility 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, several parameters were estimated. Because of this reason the databases is most applicable to Fe-based systems, i.e. steels.

Binary systems

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BCC_A2:	C-Fe	C-Cr	Cr-Fe	Cr-N	Cr-Ni	Fe-N	Fe-Ni			
FCC_A1:	Al-Cr	Al-Ni	C-Fe	C-Ni	Cr-Fe	Cr-Ni	Fe-N	Fe-Ni	Fe-Si	
HCP_A3:	C-Fe	Fe-N								
FE4N:	C-Fe	Fe-N								
Ternary syste	ems									
BCC_A2:	C-Cr-Fe									
FCC_A1:	Al-Cr-Ni C-Cr		-Fe	C-Fe-Ni						
Higher order	systems									
BCC_A2:	C-Cr-Fe-N	I-Ni								
FCC_A1:	C-Cr-Fe-N	Ji								
A model from	n Jönsson ir	ncludes th	ne effect	on diffusior	n from the	ferromagi	netic trans	ition in bo	dv-centre	2

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 is presented in the database, but since no valid diffusion model exist for liquids, a rule of thumb value of $1 \cdot 10^{-9}$ [m/s²] is used for all diffusivities. For the phase HCP_A3 most data are assumed to be the same as that in FCC_A1.

Limits

The database is primarily recommended for Fe-based alloys and steels. However, MOB2 can also be used in a few other systems, but it's important the user make sure data is indeed included for the system of interest.

Scientific Models & References

See the Thermo-Calc Software reference list and reference library at: <u>http://www.thermocalc.com/resources/</u>

www.thermocalc.com

Database acronym: N Database version: 2

MOB2 2.5