



Database name:	TCS Ni-alloys Mobility Database	Database version:	2.0
Database acronym:	MOBNi2		
Database owner:	Thermo-Calc Software AB		
Database segment:	Nickel-based superalloys		

Brief description

MOBNi2 is a kinetic database containing mobility data for Ni-based alloys 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.

MOBNi2 is compatible and primarily recommended for use in combination with the TCNi thermodynamic database.

Applications

Used together with the DICTRA software and a thermodynamic database for Ni-based alloys (e.g. TCNi), then the MOBNi2 database can be used in order to study several different phenomena of interest to Ni-based superalloys design and manufacturing, such as e.g. microsegregation during solidification, homogenisation kinetics, precipitate growth/dissolution kinetics, interdiffusion in Ni-base superalloy coating/substrate compounds, and much more.

Included Elements

Al Co Cr Fe Hf Mo Nb Ni Pd Pt Re Si Ta Ti V W Zr

Included Phases

FCC_A1 (γ) FCC_L12 (γ') BCC_A2 (α) BCC_B2 (β) LIQUID

Please note that apart from the above phases for which diffusion data are included in the database, then also other phases may be included in a DICTRA 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 DICTRA, provided a thermodynamic description for such phases has been retrieved prior to reading data from the mobility database.

Assessed Systems

FCC_A1: The database contains assessed impurity diffusion data in Ni for all included elements. It also includes complete and critical assessments for FCC_A1 in the following binary and ternary systems:

Al-Cr Al-Fe Al-Ni Co-Fe Co-Ni Co-Pd Co-Pt Cr-Fe Cr-Ni Fe-Ni Fe-Pd Fe-Pt
 Hf-Ni Mo-Ni Nb-Ni Ni-Pd Ni-Pt Ni-Re Ni-Si Ni-Ta Ni-Ti Ni-V Ni-W Ni-Zr
 Al-Cr-Ni Al-Ni-Ti Co-Fe-Ni Cr-Fe-Ni

FCC_L12: Besides the Al-Ni system itself, the diffusion of the elements listed below in Ni₃Al have been optimized and validated against experimental data. For the remaining elements some estimate based on judgement have been made.

Co Cr Fe Hf Mo Nb Pd Pt Re Si Ta Ti V

BCC_A2: This phase does normally not appear in Ni-base superalloys, at least not in any larger quantities. Even so, there is a need for a description of this phase in order to successfully model the mobilities in the ordered bcc phase. The description for this phase is based on the description available in the MOBFe1 database.

BCC_B2: For this phase several of the binary systems in which this phase is present have been optimized, e.g.

Al-Co Al-Fe Al-Ni Co-Fe Co-Ti Ni-Ti

In addition, the diffusion of the following third elements in NiAl was studied and assessed;

Co Cr Fe Mo Nb Pd Pt Ta Ti V W

LIQUID: The description present for the liquid is based on an assessment of the ternary Al-Fe-Ni system. In addition diffusivities for Mo, Re and W diffusion in Ni have been optimized, whereas remaining elements due to lack of consistent data simply is expected to diffuse like Ni.

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 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.