

## MOBNI4: TCS Ni- alloys Mobility Database

*Database name:* TCS Ni- alloys Mobility Database *Database acronym:* MOBNI

*Database owner:* Thermo-Calc Software AB *Database version:* 4.0

MOBNI4 is a kinetic database containing mobility data for Ni-based alloys 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.

MOBNI4 is compatible and primarily recommended for use in combination with the TCNI8 thermodynamic database.

### Included Elements

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

### Included Phases

FCC\_A1 ( $\gamma$ ) FCC\_L12 ( $\gamma'$ ) BCC\_A2 ( $\alpha$ ) BCC\_B2 ( $\beta$ ) 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 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

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

#### FCC\_L12

Besides the Al-Ni system itself, the diffusion of the elements listed below in Ni<sub>3</sub>Al have been optimized and validated against experimental data. For the remaining elements some estimates based on judgement are made.

B	Co	Cr	Fe	Hf	Mn	Mo	Nb	Pd	Pt	Re	Ru	Si	Ta	Ti	V
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### 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 MOBFE database.

### BCC\_B2

For this phase several of the binary systems in which this phase is present are optimized, e.g.

Al-Co	Al-Fe	Al-Ni	Co-Fe	Co-Ti	Ni-Ti
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In addition, the diffusion of the following third elements in NiAl was studied and assessed. For the remaining elements some estimates based on judgement are made.

Co	Cr	Fe	Mo	Nb	Pd	Pt	Ta	Ti	V	W
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### LIQUID

The description 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 are optimized, whereas remaining elements due to lack of consistent data 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.

### Scientific Models and References

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