# MOBNI5: TCS Ni- alloys Mobility Database

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|---|---|---|---|
| *Database name:* | TCS Ni- alloys Mobility Database | *Database acronym:* | MOBNI |
| *Database owner:* | Thermo-Calc Software AB | *Database version:* | 5.1 |

MOBNI5 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.

MOBNI5 is compatible and primarily recommended for use in combination with the TCNI9 thermodynamic database.

## Included Elements (28)

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

## Included Phases

| | | |
|---|---|---|
| FCC_A1 (γ) | FCC_L12 (γ′) | BCC_A2 (α) |
| BCC_B2 (β) | LIQUID | IONIC_LIQ |

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

## 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.

### Binary

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 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 | | |

### Ternary

| | | | | | | |
|---|---|---|---|---|---|---|
| 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 Ni3Al 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 |

## 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 |

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 |

### 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. The diffusivities of Ca, Mg and S are estimated using the modified Sutherland equation, 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 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/.