The TCNI database

Nathalie Dupin

Calcul Thermodynamique

Outline

- Generalities
- fcc
  - Ordering
  - MC
- bcc
  - Ordering
  - 2nd order
- Conclusion
Commercial thermodynamic Database developed by TCSAB in the framework of a collaboration with industrial partners to describe the phase equilibria in the Ni base superalloys.

J. Bratberg et al. Superalloys 2012
TCNI

- Commercial thermodynamic Database developed by TCSAB in the framework of a collaboration with industrial partners to describe the phase equilibria in the Ni base superalloys.

- All the binary systems constituting the complex system Al-B-C-Co-Cr-Fe-Hf-Mn-Mo-N-Nb-Ni-O-Pd-Pt-Re-Ru-Si-Ta-Ti-V-W-Y-Zr are described.
Commercial thermodynamic Database developed by TCSAB in the framework of a collaboration with industrial partners to describe the phase equilibria in the Ni base superalloys.

All the binary system constituting the complex system Al-B-C-Co-Cr-Fe-Hf-Mn-Mo-N-Nb-Ni-O-Pd-Pt-Re-Ru-Si-Ta-Ti-V-W-Y-Zr are described.

Only the phases of interest for the industrial alloys are extracted by default.

When the database is selected, the list of all the phases rejected by default is displayed.

The user can of course restore the phases of interest for any calculation.
Commercial thermodynamic Database developed by TCSAB in the framework of a collaboration with industrial partners to describe the phase equilibria in the Ni base superalloys.

All the binary systems constituting the complex system Al-B-C-Co-Cr-Fe-Hf-Mn-Mo-N-Nb-Ni-O-Pd-Pt-Re-Ru-Si-Ta-Ti-V-W-Y-Zr are described.

Only the phases of interest for the industrial alloys are extracted by default.

The description of all the binary systems and of many assessed ternary systems are available using the BINARY and TERNARY modules.
Commercial thermodynamic Database developed by TCSAB in the framework of a collaboration with industrial partners to describe the phase equilibria in the Ni base superalloys.

All the binary system constituting the complex system Al-B-C-Co-Cr-Fe-Hf-Mn-Mo-N-Nb-Ni-O-Pd-Pt-Re-Ru-Si-Ta-Ti-V-W-Y-Zr are described.

Only the phases of interest for the industrial alloys are extracted by default.

The description of all the binary systems and of many assessed ternary systems are available using the BINARY and TERNARY modules.

This database uses a single equation to model the $A_1/L_1$ on the one hand and $A_2/B_2$ on the other hand that show ordering crystallographic relationship.
fcc ordering

go bin
TCNI
Al
Ni
fcc ordering

go bin
TCNI
Al
Ni
fcc ordering

go bin
TCNI
Al
Ni
fcc ordering

go bin
TCNI
Al
Ni

back
go poly
list_cond
read,,
set_cond x(ni)=.8 t=1200
compute_eq
list_eq
fcc ordering

```
POLY_3: le
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label AO , database: USER

Conditions:
X(NI)=0.8, P=1E5, N=1, T=1200
DEGREES OF FREEDOM 0

Temperature 1200.00 K (926.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.23484E+01
Total Gibbs energy -8.75017E+04, Enthalpy -5.40654E+03, Volume 7.08284E-06

Component Moles W-Fraction Activity Potential Ref.stat
AL 2.0000E-01 1.0309E-01 1.7170E-06 -1.3245E+05 FCC_A1
NI 8.0000E-01 8.9691E-01 6.8371E-01 -3.7936E+03 FCC_A1

FCC_L12#2 ORD Status ENTERED Driving force 0.0000E+00
Moles 6.3732E-01, Mass 3.2734E+01, Volume fraction 6.4022E-01 Mass fractions:
NI 8.79167E-01 AL 1.20833E-01

FCC_L12 DISORD Status ENTERED Driving force 0.0000E+00
Moles 3.6268E-01, Mass 1.9593E+01, Volume fraction 3.5978E-01 Mass fractions:
NI 9.26579E-01 AL 7.34214E-02
```
fcc ordering

```
POLY_3: l_e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /WVCS/:

Output from POLY-3, equilibrium = 1, label AO, database: USER

Conditions:
X(NI)=0.8, P=1E5, N=1, T=1200
DEGREES OF FREEDOM 0

Temperature 1200.00 K (926.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.23484E+01
Total Gibbs energy -8.75017E+04, Enthalpy -5.40654E+03, Volume 7.08284E-06

Component Moles W-Fraction Activity Potential Ref.stat
AL 2.0000E-01 1.0309E-01 1.7170E-06 -1.3245E+05 FCC_A1
NI 8.0000E-01 8.9691E-01 6.8371E-01 -3.7936E+03 FCC_A1

FCC_L12#2 ORD Status ENTERED Driving force 0.0000E+00
Moles 6.3732E-01, Mass 3.2754E+01, Volume fraction 6.4022E-01 Mass fractions:
NI 8.79167E-01 AL 1.20833E-01
Constitution:
Sublattice 1, Number of sites 7.5000E-01
NI 9.95375E-01 AL 4.62502E-03
Sublattice 2, Number of sites 2.5000E-01
AL 9.06726E-01 NI 9.32742E-02
Sublattice 3, Number of sites 1.0000E+00
VA 1.00000E+00

FCC_L12 DISORD Status ENTERED Driving force 0.0000E+00
Moles 3.6268E-01, Mass 1.9595E+01, Volume fraction 3.5978E-01 Mass fractions:
NI 9.26579E-01 AL 7.34214E-02
Constitution:
Sublattice 1, Number of sites 7.5000E-01
NI 8.52982E-01 AL 1.47018E-01
Sublattice 2, Number of sites 2.5000E-01
NI 8.52982E-01 AL 1.47018E-01
Sublattice 3, Number of sites 1.0000E+00
VA 1.00000E+00
```
fcc ordering

\[
\text{POLY}_3:\_e
\]
\[
\text{OUTPUT TO SCREEN OR FILE } /\text{SCREEN}/:
\]
\[
\text{Options } /\text{WVCS}/:\n\]
\[
\text{Output from POLY-3, equilibrium } = 1, \text{ label AO }, \text{ database: USER}
\]

Conditions:
\[
X(\text{NI})=0.8, \text{ P}=1E5, \text{ N}=1, \text{ T}=1200
\]
\[
\text{DEGREES OF FREEDOM 0}
\]

Temperature 1200.00 K (926.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.23484E+01
Total Gibbs energy -8.75017E+04, Enthalpy -5.40654E+03, Volume 7.08284E-06

Component \hspace{1cm} Moles \hspace{1cm} W-Fraction \hspace{1cm} Activity \hspace{1cm} Potential \hspace{1cm} Ref.stat
\[
\text{AL} \hspace{1cm} 2.0000E-01 \hspace{1cm} 1.0309E-01 \hspace{1cm} 1.7170E-06 \hspace{1cm} -1.3245E+05 \hspace{1cm} \text{FCC}_A1
\]
\[
\text{NI} \hspace{1cm} 8.0000E-01 \hspace{1cm} 8.9691E-01 \hspace{1cm} 6.8371E-01 \hspace{1cm} -3.7936E+03 \hspace{1cm} \text{FCC}_A1
\]

FCC\_L12\#2 \hspace{1cm} ORD \hspace{1cm} Status ENTERED \hspace{1cm} Driving force 0.0000E+00
Moles 6.3732E-01, Mass 3.2754E+01, Volume fraction 6.4022E-01 Mass fractions:
\[
\text{NI} \hspace{1cm} 8.79167E-01 \hspace{1cm} \text{AL} \hspace{1cm} 1.20833E-01
\]

Constitution:
\[
\text{Sublattice 1, Number of sites 7.5000E-01}
\]
\[
\text{NI} \hspace{1cm} 9.95375E-01 \hspace{1cm} \text{AL} \hspace{1cm} 4.62502E-03
\]
\[
\text{Sublattice 2, Number of sites 2.5000E-01}
\]
\[
\text{AL} \hspace{1cm} 9.06726E-01 \hspace{1cm} \text{NI} \hspace{1cm} 9.32742E-02
\]
\[
\text{Sublattice 3, Number of sites 1.0000E+00}
\]
\[
\text{VA} \hspace{1cm} 1.00000E+00
\]

FCC\_L12 \hspace{1cm} DISORD \hspace{1cm} Status ENTERED \hspace{1cm} Driving force 0.0000E+00
Moles 3.6268E-01, Mass 1.9595E+01, Volume fraction 3.5978E-01 Mass fractions:
\[
\text{NI} \hspace{1cm} 9.26579E-01 \hspace{1cm} \text{AL} \hspace{1cm} 7.34214E-02
\]

Constitution:
\[
\text{Sublattice 1, Number of sites 7.5000E-01}
\]
\[
\text{NI} \hspace{1cm} 8.52982E-01 \hspace{1cm} \text{AL} \hspace{1cm} 1.47018E-01
\]
\[
\text{Sublattice 2, Number of sites 2.5000E-01}
\]
\[
\text{NI} \hspace{1cm} 8.52982E-01 \hspace{1cm} \text{AL} \hspace{1cm} 1.47018E-01
\]
\[
\text{Sublattice 3, Number of sites 1.0000E+00}
\]
\[
\text{VA} \hspace{1cm} 1.00000E+00
\]
fcc ordering

POLY_3; l_e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /WVCS/:
Output from POLY-3, equilibrium = 1, label AO , database: USER

Conditions:
X(NI)=0.8, P=1E5, N=1, T=1200
DEGREES OF FREEDOM 0

Temperature 1200.00 K (926.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.23484E+01
Total Gibbs energy -8.75017E+04, Enthalpy -5.40654E+03, Volume 7.08284E-06

Component Moles W-Fraction Activity Potential Ref.stat
AL 2.0000E-01 1.0309E-01 1.7170E-06 -1.3245E+05 FCC_A1
NI 8.0000E-01 8.9691E-01 6.8371E-01 -3.7936E+03 FCC_A1

FCC_L12#2 ORD Status ENTERED Driving force 0.0000E+00
Moles 6.3732E-01, Mass 3.2754E+01, Volume fraction 6.4022E-01 Mass fractions:
NI 8.79167E-01 AL 1.20833E-01

Constitution:
Sublattice 1, Number of sites 7.5000E-01
NI 9.95375E-01 AL 4.62502E-03
Sublattice 2, Number of sites 2.5000E-01
AL 9.06726E-01 NI 9.32742E-02
Sublattice 3, Number of sites 1.0000E+00
VA 1.00000E+00

FCC_L12 DISORD Status ENTERED Driving force 0.0000E+00
Moles 3.62688E-01, Mass 1.95955E+01, Volume fraction 3.5978E-01 Mass fractions:
NI 9.26579E-01 AL 7.34214E-02

Constitution:
Sublattice 1, Number of sites 7.5000E-01
NI 8.52982E-01 AL 1.47018E-01
Sublattice 2, Number of sites 2.5000E-01
NI 8.52982E-01 AL 1.47018E-01
Sublattice 3, Number of sites 1.0000E+00
VA 1.00000E+00
fcc ordering

\[
\begin{align*}
\text{POLY}_3: & \text{ \_e} \\
\text{OUTPUT TO SCREEN OR FILE /SCREEN/;} \\
\text{Options /WVCS/:} & \text{n} \\
\text{Output from POLY-3, equilibrium = 1, label AO, database: USER} \\
\text{Conditions:} \\
X(\text{Ni}) &= 0.8, P=1E5, N=1, T=1200 \\
\text{DEGREES OF FREEDOM 0} \\
\text{Temperature} & = 1200.00 \text{ K (926.85 C), Pressure} = 1.000000E+05 \\
\text{Number of moles of components} & = 1.000000E+00, \text{Mass in grams} = 5.23484E+01 \\
\text{Total Gibbs energy} & = -8.75017E+04, \text{Enthalpy} = -5.40654E+03, \text{Volume} = 7.08284E-06 \\
\text{Component} & \quad \text{Moles} \quad \text{W-Fraction} \quad \text{Activity} \quad \text{Potential} \quad \text{Ref.stat} \\
\text{AL} & \quad 2.0000E-01 \quad 1.0309E-01 \quad 1.7170E-06 \quad -1.3245E+05 \quad \text{FCC\_A1} \\
\text{NI} & \quad 8.0000E-01 \quad 8.9691E-01 \quad 6.8371E-01 \quad -3.7936E+03 \quad \text{FCC\_A1} \\
\text{FCC\_L12\#2} & \quad \text{ORD Status ENTERED} \quad \text{Driving force} = 0.0000E+00 \\
\text{Moles} & = 6.3732E-01, \text{Mass} = 3.2754E+01, \text{Volume fraction} = 6.4022E-01 \quad \text{Mass fractions:} \\
\text{NI} & = 8.7916E-01 \quad \text{AL} = 1.20833E-01 \\
\text{Constitution:} \\
\text{Sublattice 1, Number of sites} & = 7.5000E-01 \\
\text{NI} & = 9.95375E-01 \quad \text{AL} = 4.62502E-03 \\
\text{Sublattice 2, Number of sites} & = 2.5000E-01 \\
\text{NI} & = 9.06726E-01 \quad \text{AL} = 9.32742E-02 \\
\text{Sublattice 3, Number of sites} & = 1.0000E+00 \\
\text{VA} & = 1.00000E+00 \\
\text{FCC\_L12} & \quad \text{DISORD Status ENTERED} \quad \text{Driving force} = 0.0000E+00 \\
\text{Moles} & = 3.6268E-01, \text{Mass} = 1.9595E+01, \text{Volume fraction} = 3.5978E-01 \quad \text{Mass fractions:} \\
\text{NI} & = 9.26579E-01 \quad \text{AL} = 7.34214E-02 \\
\text{Constitution:} \\
\text{Sublattice 1, Number of sites} & = 7.5000E-01 \\
\text{NI} & = 8.52982E-01 \quad \text{AL} = 1.47018E-01 \\
\text{Sublattice 2, Number of sites} & = 2.5000E-01 \\
\text{NI} & = 8.52982E-01 \quad \text{AL} = 1.47018E-01 \\
\text{Sublattice 3, Number of sites} & = 1.0000E+00 \\
\text{VA} & = 1.00000E+00
\end{align*}
\]

\[
\begin{align*}
(\text{Al}_{0.005}\text{Ni}_{0.995})^{0.75} \\
(\text{Al}_{0.907}\text{Ni}_{0.093})^{0.25} \\
(\text{Al}_{0.147}\text{Ni}_{0.853})^{0.75} \\
(\text{Al}_{0.147}\text{Ni}_{0.853})^{0.25}
\end{align*}
\]
fcc ordering

Plot 1

2016.09.28.18.29.47
USER: AL, Ni
P=1E5, N=1

AL Ni

1: FCC_L12 DISORD
2: FCC_L12#2 ORD
3: LIQUID
4: BCC_B2#2 ORD
go bin
go bin
Ti C
MC

go bin
TCNI
Ti C

back
go poly
list_cond
read,,
set_cond x(ti)=.6
compute_eq
list_eq

N
go bin
TCNI
Ti C

back

go poly
list_cond
read,
set_cond x(t)i= .6
compute_eq
list_eq
N

Output from POLY-3, equilibrium =  1, label AO , database: USER

Conditions:
X(Ti)=0.6, P=1E5, N=1, T=1200
DEGREES OF FREEDOM 0

Temperature  1200.00 K ( 926.85 C), Pressure 1.000000E+05
Number of moles of components  1.000000E+00, Mass in grams 3.35324E+01
Total Gibbs energy -1.16840E+05, Enthalpy -4.78829E+04, Volume 7.45017E-06

Component  Moles  W-Fraction  Activity  Potential  Ref.stat
C     4.0000E-01  1.4328E-01  1.2580E-07  -1.5853E+05  GRAPHITE
TI    6.0000E-01  8.5672E-01  1.5537E-01  -1.8577E+04  HCP_A3

FCC_L12       DISORD Status ENTERED  Driving force 0.0000E+00
Moles 1.0000E+00, Mass 3.35324E+01, Volume fraction 1.0000E+00  Mass fractions:
TI  8.56724E-01  C  1.43276E-01

Constitution:
Sublattice 1, Number of sites  7.5000E-01 (Ti)0.75
TI  1.00000E+00
Sublattice 2, Number of sites  2.5000E-01 (Ti)0.25
TI  1.00000E+00
Sublattice 3, Number of sites  1.0000E+00 (C0.666□0.333)
C  6.66667E-01  VA  3.33333E-01
The FCC_L12 phase also describes the cubic carbides of MC type when the last sublattice contains an important fraction of C.
Al-Ni-Ti-C

```
go data
sw TCNI
def_sy Al Ni Ti C
get
go pol
s_c p=1E5 n=1 t=1200
s_c x(Al)=.05 x(Ti)=.1
s_c x(C)=.01
```
Al-Ni-Ti-C

```
go data
sw TCNI
def_sy Al Ni Ti C
get
go pol
s_c p=1E5 n=1 t=1200
s_c x(Al)=.05 x(Ti)=.1
s_c x(C)=.01
```

Conditions:
P=1E5, T=1200, N=1, X(Al)=5E-2, X(Ti)=0.1, X(C)=1E-2
DEGREES OF FREEDOM 0

Temperature 1200.00 K ( 926.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.55568E+01
Total Gibbs energy -8.09479E+04, Enthalpy 6.46171E+03, Volume 7.11465E-06

Component Moles W-Fraction Activity Potential Ref.stat
AL 5.0000E-02 2.4283E-02 8.1339E-10 -2.0883E+05 SER
C 1.0000E-02 2.1619E-03 1.1936E-02 -4.4182E+04 SER
NI 6.4000E-01 8.8737E-01 2.1343E-30 -6.1357E+04 SER
TI 1.0000E-01 8.6182E-02 8.6040E-09 -1.8525E+05 SER

FCC_L12#2 DISORD Status ENTERED Driving force 0.00000E+00
Moles 6.4369E-01, Mass 3.5583E+01, Volume Fration 6.3940E-01 Mass fractions:
Constitution:
Sublattice 1, Number of sites 7.50000E-01
NI 8.91595E-01 TI 7.90144E-02 AL 2.93907E-02
Sublattice 2, Number of sites 2.50000E-01
NI 8.91595E-01 TI 7.90144E-02 AL 2.93907E-02
Sublattice 3, Number of sites 1.00000E+00
VA 9.98428E-01 C 1.57191E-03

FCC_L12#3 ORD Status ENTERED Driving force 0.00000E+00
Moles 3.3974E-01, Mass 1.8468E+01, Volume Fraction 3.4556E-01 Mass fractions:
NI 8.48504E-01 TI 1.05406E-01 AL 4.54552E-02 C 6.35238E-04
Constitution:
Sublattice 1, Number of sites 7.50000E-01
NI 9.99873E-01 AL 8.02817E-05 TI 4.69657E-05
Sublattice 2, Number of sites 2.50000E-01
TI 4.79911E-01 AL 3.67115E-01 NI 1.52974E-01
Sublattice 3, Number of sites 1.00000E+00
VA 9.97117E-01 C 2.88321E-03

FCC_L12 DISORD Status ENTERED Driving force 0.00000E+00
Moles 1.6578E-02, Mass 5.0634E-01, Volume Fraction 1.5036E-02 Mass fractions:
TI 8.09804E-01 C 1.90079E-01 NI 1.16846E-04 AL 1.16538E-11
Constitution:
Sublattice 1, Number of sites 7.50000E-01
TI 9.99882E-01 NI 1.17698E-04 AL 2.55338E-11
Sublattice 2, Number of sites 2.50000E-01
TI 9.99882E-01 NI 1.17698E-04 AL 2.55338E-11
Sublattice 3, Number of sites 1.00000E+00
C 9.35573E-01 VA 6.44271E-02
Al-Ni-Ti-C

go data
sw TCNI
def_sy Al Ni Ti C
get
s_c p=1E5 n=1 t=1200
s_c x(Al)=.05 x(Ti)=.1
s_c x(C)=.01

The FCC_L12 phase describes

− $\gamma$, A1
− $\gamma'$, L1$_2$
− MC, B1.

Nathalie Dupin (CThermo)

TCNI
bcc ordering

go ter
TCNI
Ni Cr Al
### bcc ordering

**go ter**  
TCNI  
Ni Cr Al

### sto

<table>
<thead>
<tr>
<th>Component</th>
<th>Moles</th>
<th>W-Fraction</th>
<th>Activity</th>
<th>Potential</th>
<th>Ref.stat</th>
</tr>
</thead>
<tbody>
<tr>
<td>AL</td>
<td>4.0000E-01</td>
<td>2.3806E-01</td>
<td>8.9482E-07</td>
<td>-1.4742E+05</td>
<td>SER</td>
</tr>
<tr>
<td>CR</td>
<td>1.0000E-01</td>
<td>1.1469E-01</td>
<td>6.4766E-03</td>
<td>-5.3347E+04</td>
<td>SER</td>
</tr>
<tr>
<td>NI</td>
<td>5.0000E-01</td>
<td>6.4726E-01</td>
<td>2.1100E-04</td>
<td>-8.9593E+04</td>
<td>SER</td>
</tr>
</tbody>
</table>

**BCC_B2#2**  
ORD Status ENTERED  
Driving force 0.0000E+00

Mass fractions:

<table>
<thead>
<tr>
<th>Component</th>
<th>Moles</th>
<th>W-Fraction</th>
<th>Activity</th>
<th>Potential</th>
</tr>
</thead>
<tbody>
<tr>
<td>NI 6.9128E-01</td>
<td>AL 2.54176E-01</td>
<td>CR 5.45440E-02</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**BCC_B2**  
DISORD Status ENTERED  
Driving force 0.0000E+00

Moles 5.6639E-02, Mass 2.9348E+00, Volume fraction 5.6194E-02
Mass fractions:

<table>
<thead>
<tr>
<th>Component</th>
<th>Moles</th>
<th>W-Fraction</th>
<th>Activity</th>
<th>Potential</th>
</tr>
</thead>
<tbody>
<tr>
<td>CR 9.83643E-01</td>
<td>NI 1.12237E-02</td>
<td>AL 5.13316E-03</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Constitution:**

- **Sublattice 1**, Number of sites 5.0000E-01
- **Sublattice 2**, Number of sites 5.0000E-01
- **Sublattice 3**, Number of sites 3.0000E+00
bcc ordering

go ter
TCNI
Ni Cr Al

b
go pol
l_c
rea.,,
s_c x(cr)=.1
s_c x(ni)=.5
c_e
l_e

Nathalie Dupin (CThermo)
The BCC_B2 phase describes

- B2, the AlNi compound.
- A2, the Cr based solid solution.

The BCC_B2 phase describes

- B2, the AlNi compound.
- A2, the Cr based solid solution.
2nd order transition

go ter
TCNI
Co Cr Al

1300
2nd order transition

go ter
TCNI
Co Cr Al

1300

... There is a field where the transition between the B2 ordered phase and the A2 disordered phase occurs continuously, without A2+B2 two phase field.
There is a field where the transition between the B2 ordered phase and the A2 disordered phase occurs continuously, without A2+B2 two phase field.

It is called a second order transition as, for a given composition, during heating, there is no noticeable effect on $H$, first derivative of $G$, but for the le $C_p$, second derivative.
2nd order transition

go ter
TCNI
Co Cr Al

1300

... There is a field where the transition between the B2 ordered phase and the A2 disordered phase occurs continuously, without A2+B2 two phase field.

It is called a second order transition as, for a given composition, during heating, there is no noticeable effect on $H$, first derivative of $G$, but for the le $C_p$, second derivative.

It is also called a $\lambda$ transition, due to the shape of the $C_p$ curve during such a transition.
2nd order transition

go te
TCNI
Co Cr Al

1300

... 

There is a field where the transition between the B2 ordered phase and the A2 disordered phase occurs continuously, without A2+B2 two phase field.

It is called a second order transition as, for a given composition, during heating, there is no noticeable effect on H, first derivative of G, but for the le Cp, second derivative.

It is also called a \(\lambda\) transition, due to the shape of the Cp curve during such a transition.

The way to calculate such a transition is showed in the Fe-Al binary case by tcex16 example.
Conclusion

- The commercial thermodynamic database TCNI allows to calculate multicomponent equilibria of interest in the field of Ni base superalloys.

- It is characterized by
  - a complete description of all the constitutive binary systems, allowing calculations for simplified compositions or very far from usual industrial alloys,
  - a thermodynamic description taking into account the ordering relationships between the phases A1/L1\textsubscript{2} and A2/B2, allowing in particular to describe the second order transition of these latter.