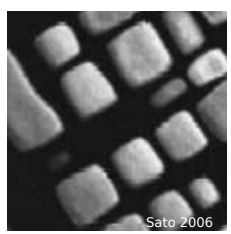
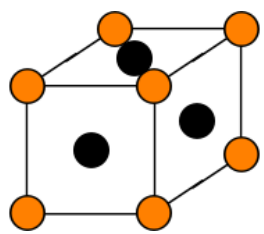
The TCNI database

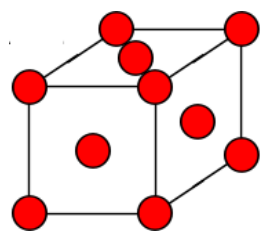
Nathalie Dupin

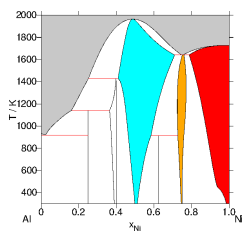
Calcul Thermodynamique

Paris, Ecole des Mines, 20 oct. 2016







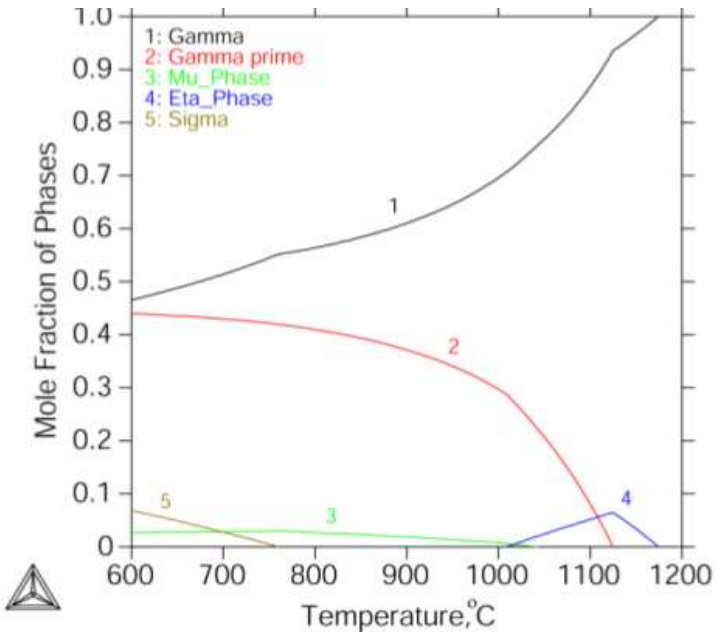


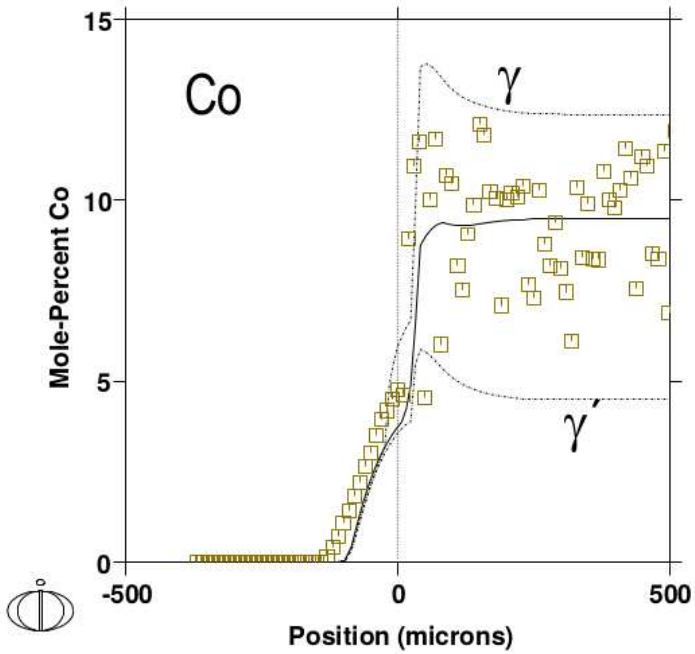
Outline

- Generalities
- fcc
  - Ordering
  - MC
- bcc
  - Ordering
  - 2nd order
- Conclusion

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 .

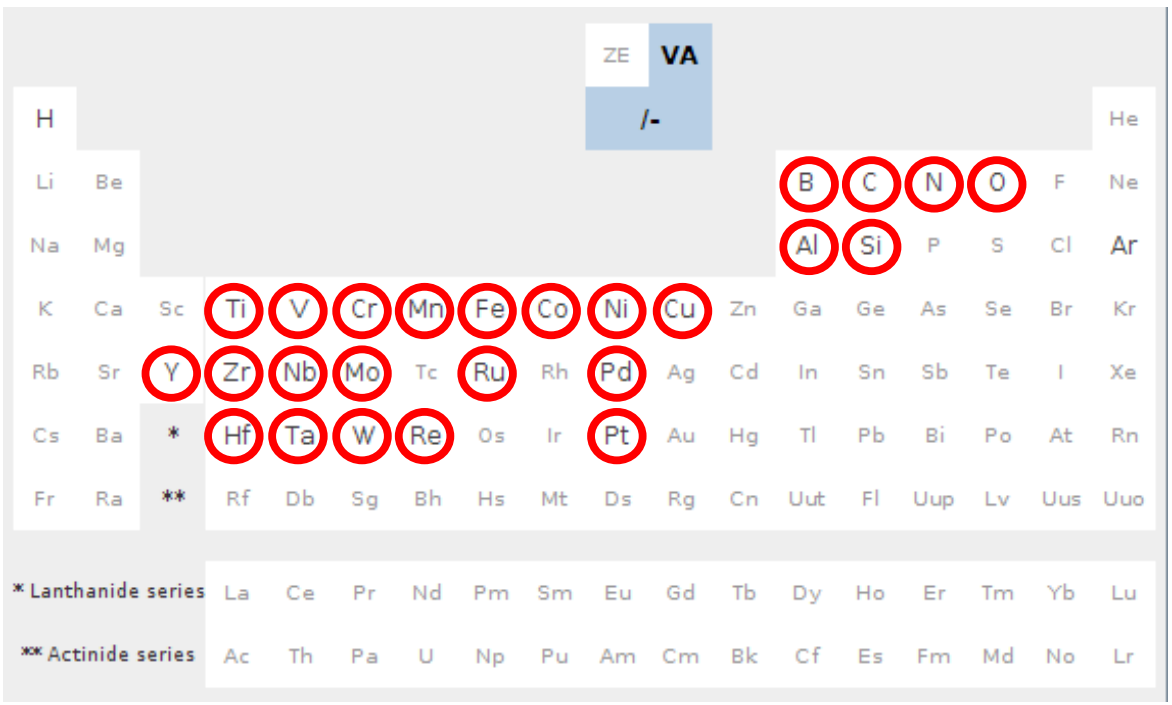




J. Bratberg *et al.* Superalloys 2012

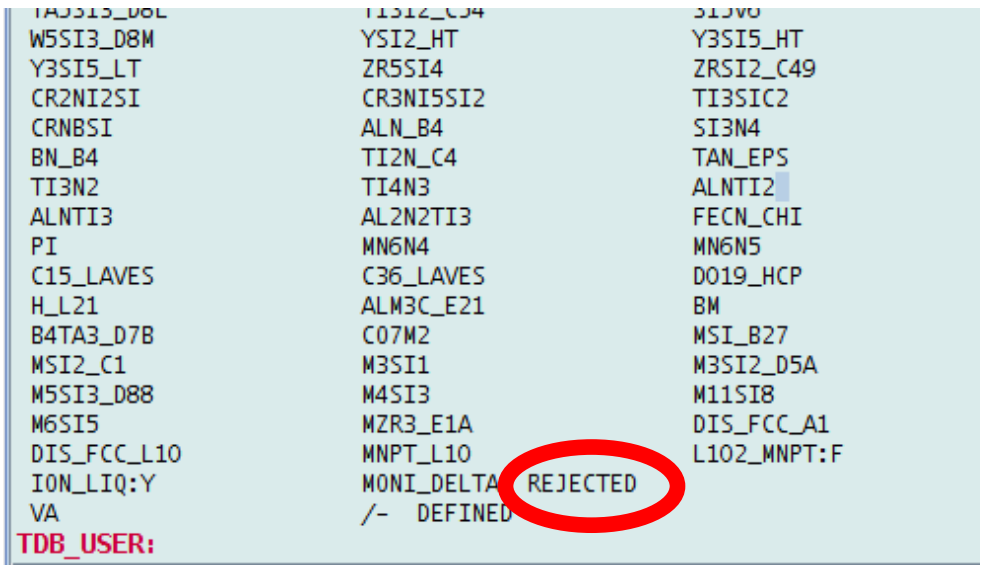
TCNI

- 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 system consituting 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.



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 system consituting 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.

TCNI

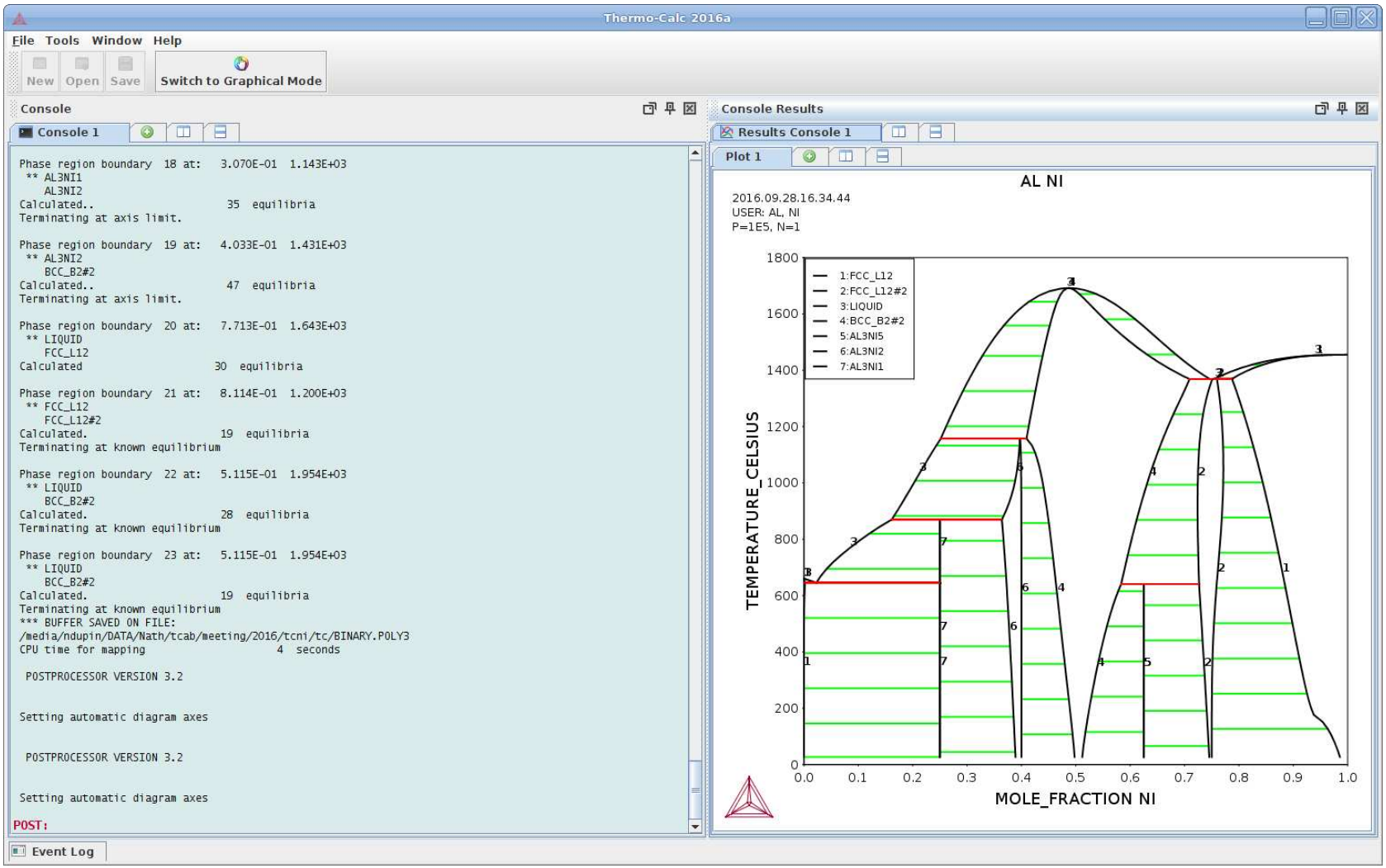
- Commercial thermodynamic Database developed by TCSAB in the framework of a collaboration with industrial partners to describe the phase equilibria in the Ni base superalloys .
- All the binary system consituting the complex system Al-B-C-Co -Cr-Fe-Hf-Mn-Mo-N-Nb-Ni-O-Pd-Pt-Re-Ru-Si-Ta-Ti-V-W-Y-Zr are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

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 system consituting 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 $A1/L1_2$ on the one hand and $A2/B2$ on the other hand that show ordering cristallographic relationship.

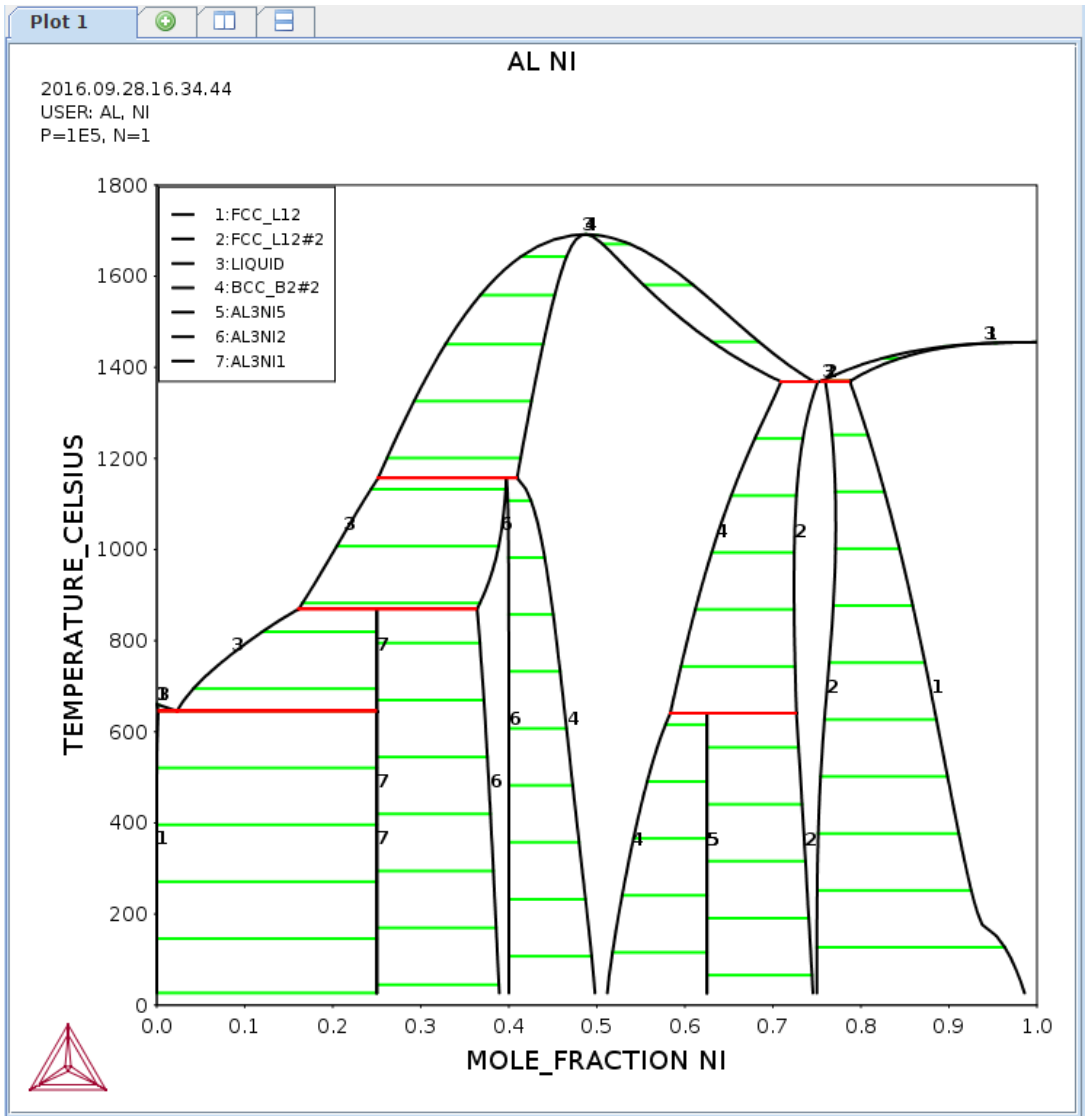
fcc ordering

```
go bin
TCNI
Al
Ni
```



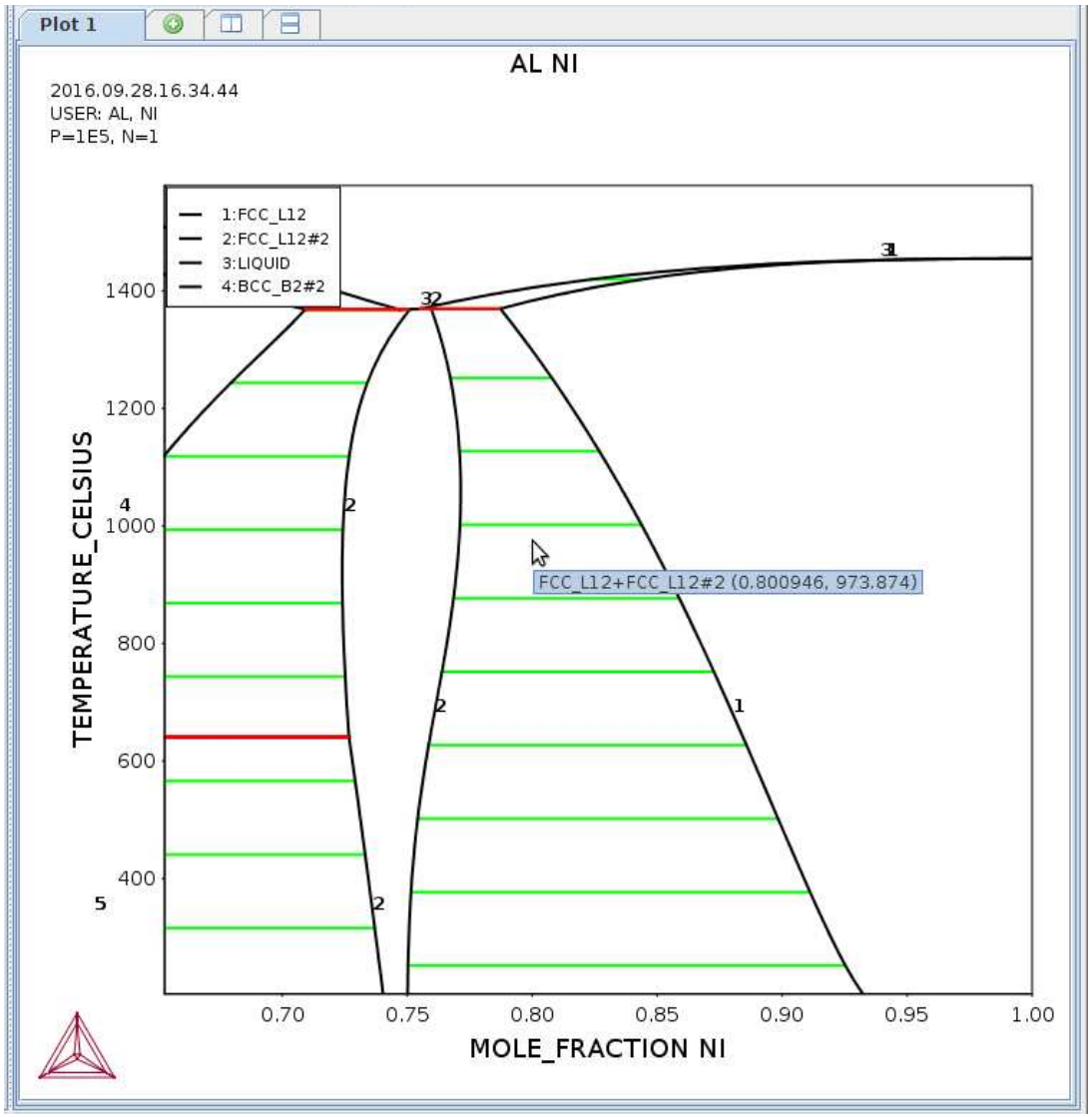
fcc ordering

```
go bin
TCNI
Al
Ni
```



fcc ordering

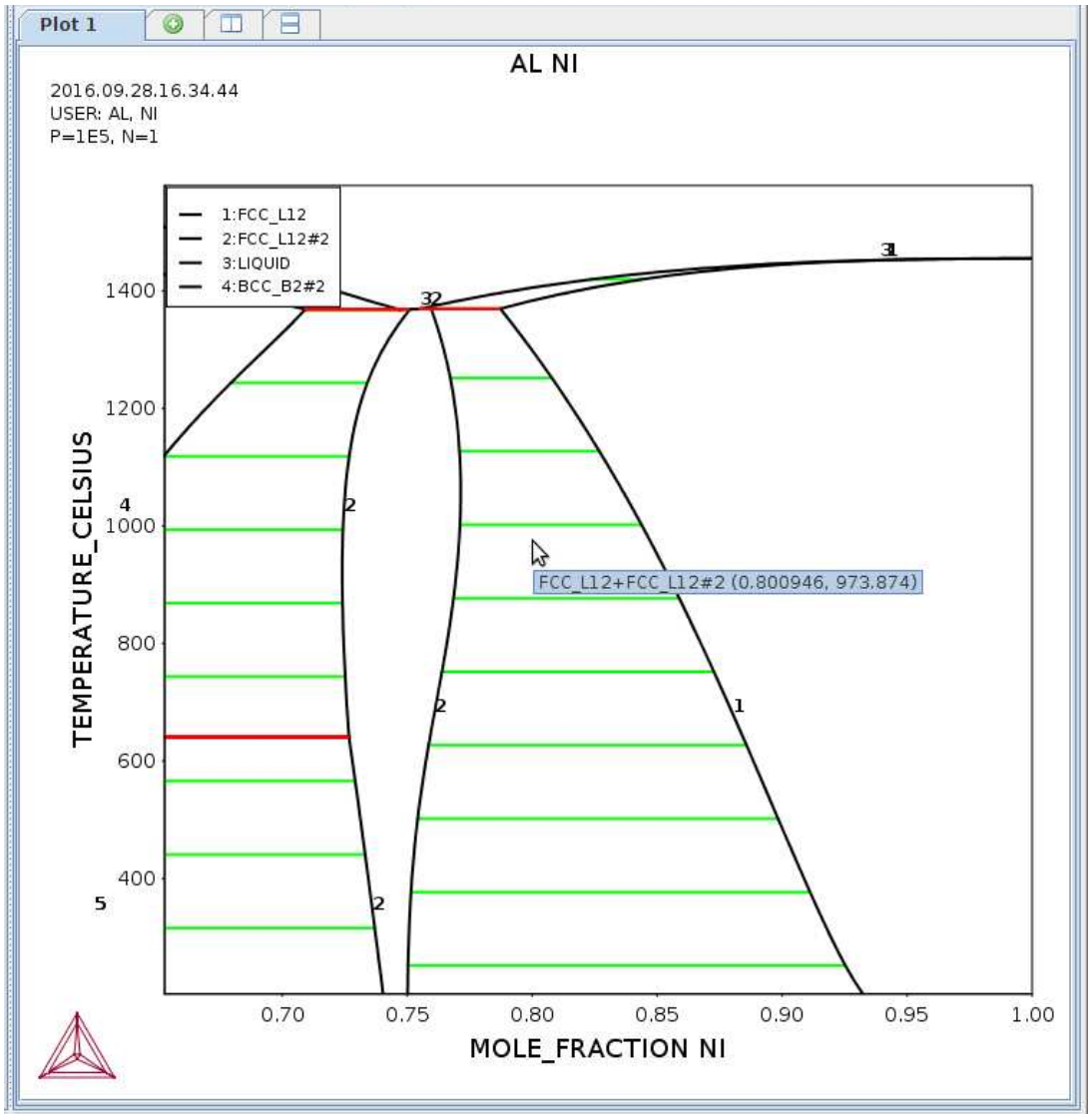
```
go bin
TCNI
Al
Ni
```



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:l_e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
 Output from POLY-3, equilibrium =     1, label A0  , 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  1.00000E+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

 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
```

fcc ordering

```
l_e

N
```

```
POLY_3:l_e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:n
 Output from POLY-3, equilibrium =     1, label A0  , 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  1.00000E+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

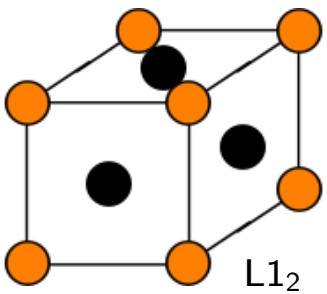
 FCC_L12#2                ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 6.3732E-01, Mass 3.2754E+01, Volume fraction 6.4022E-01  Mass fractions:
 NI  8.79167E-01  AL  1.20833E-01
 Constitution:
 Sublattice  1,  Number of sites  7.5000E-01
 NI  9.95375E-01  AL  4.62502E-03
 Sublattice  2,  Number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

```
l_e

N
```




```
POLY_3:l_e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:n
 Output from POLY-3, equilibrium =     1, label A0  , 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  1.00000E+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

```
l_e

N
```

```
POLY_3:l_e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:n
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

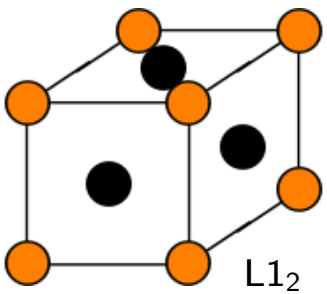
 Conditions:
 X(NI)=0.8, P=1E5, N=1, T=1200
 DEGREES OF FREEDOM 0

 Temperature   1200.00 K (   926.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.23484E+01
 Total Gibbs energy -8.75017E+04,  Enthalpy -5.40654E+03,  Volume  7.08284E-06

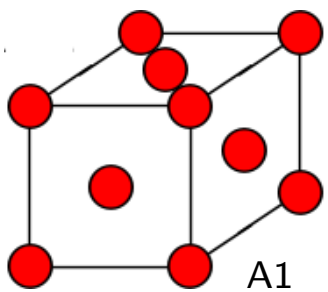
 Component              Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                     2.0000E-01  1.0309E-01 1.7170E-06 -1.3245E+05 FCC_A1
 NI                     8.0000E-01  8.9691E-01 6.8371E-01 -3.7936E+03 FCC_A1

 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
```



$L1_2$



A1

fcc ordering

```
l_e

N
```

```
POLY_3:l_e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:n
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

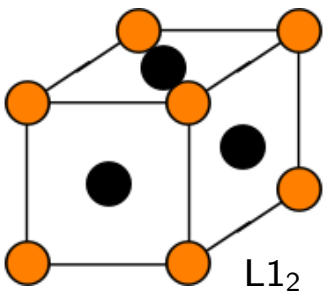
 Conditions:
 X(NI)=0.8, P=1E5, N=1, T=1200
 DEGREES OF FREEDOM 0

 Temperature   1200.00 K (   926.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+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
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 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

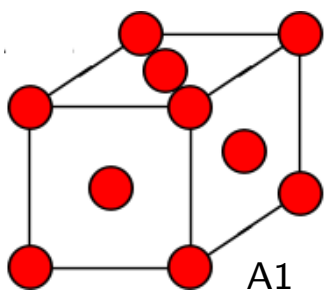
 FCC_L12                 DISORD Status ENTERED   Driving force  0.0000E+00
 Moles 3.6268E-01, Mass 1.9595E+01, Volume fraction 3.5978E-01  Mass fractions:
 NI  9.26579E-01  AL  7.34214E-02
 Constitution:
 Sublattice  1,  Number of sites  7.5000E-01
 NI  8.52982E-01  AL  1.47018E-01
 Sublattice  2,  Number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



$L1_2$

$(Al_{0.005}Ni_{0.995})_{0.75}$

$(Al_{0.907}Ni_{0.093})_{0.25}$



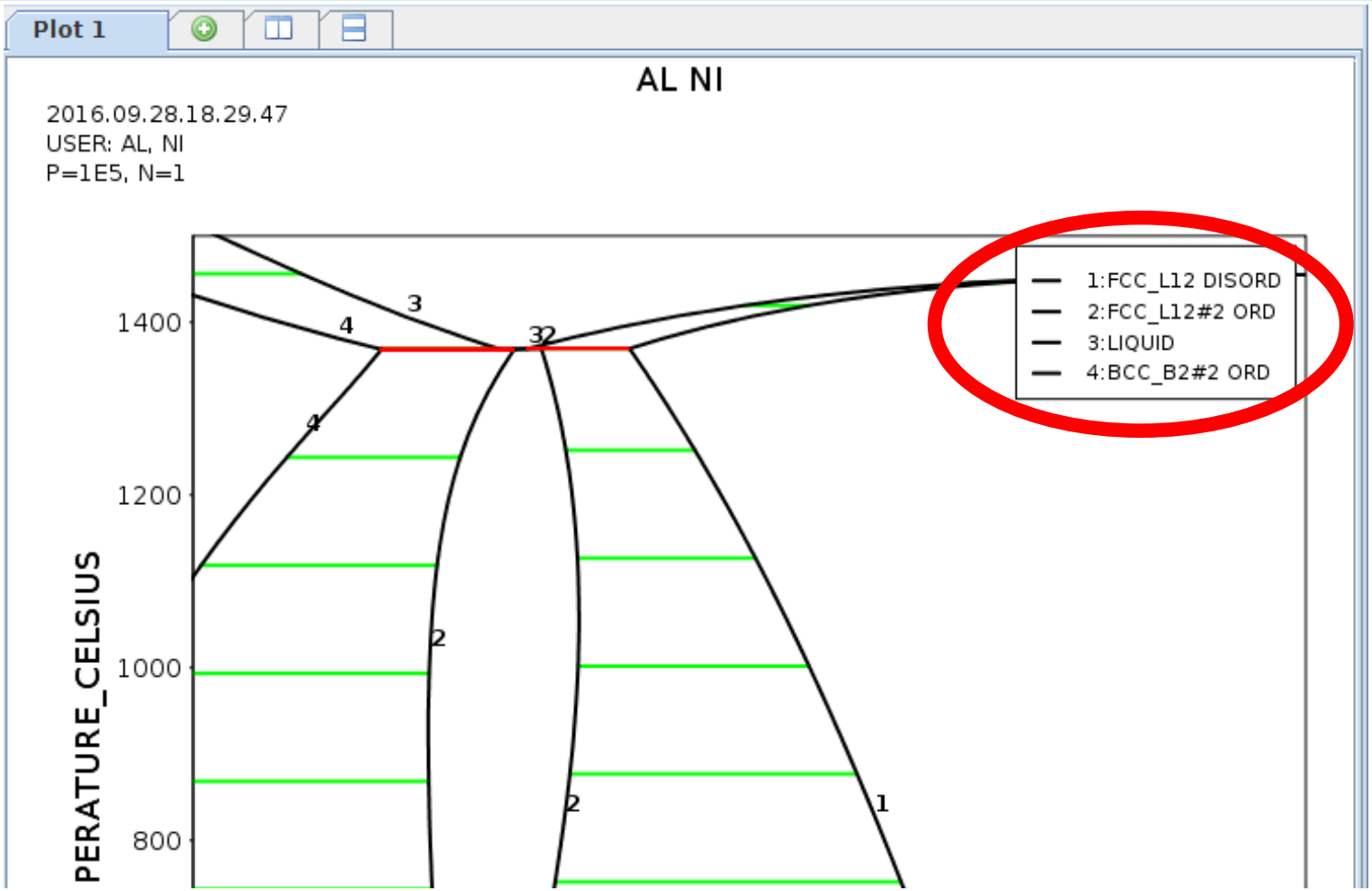
A1

$(Al_{0.147}Ni_{0.853})_{0.75}$

$(Al_{0.147}Ni_{0.853})_{0.25}$

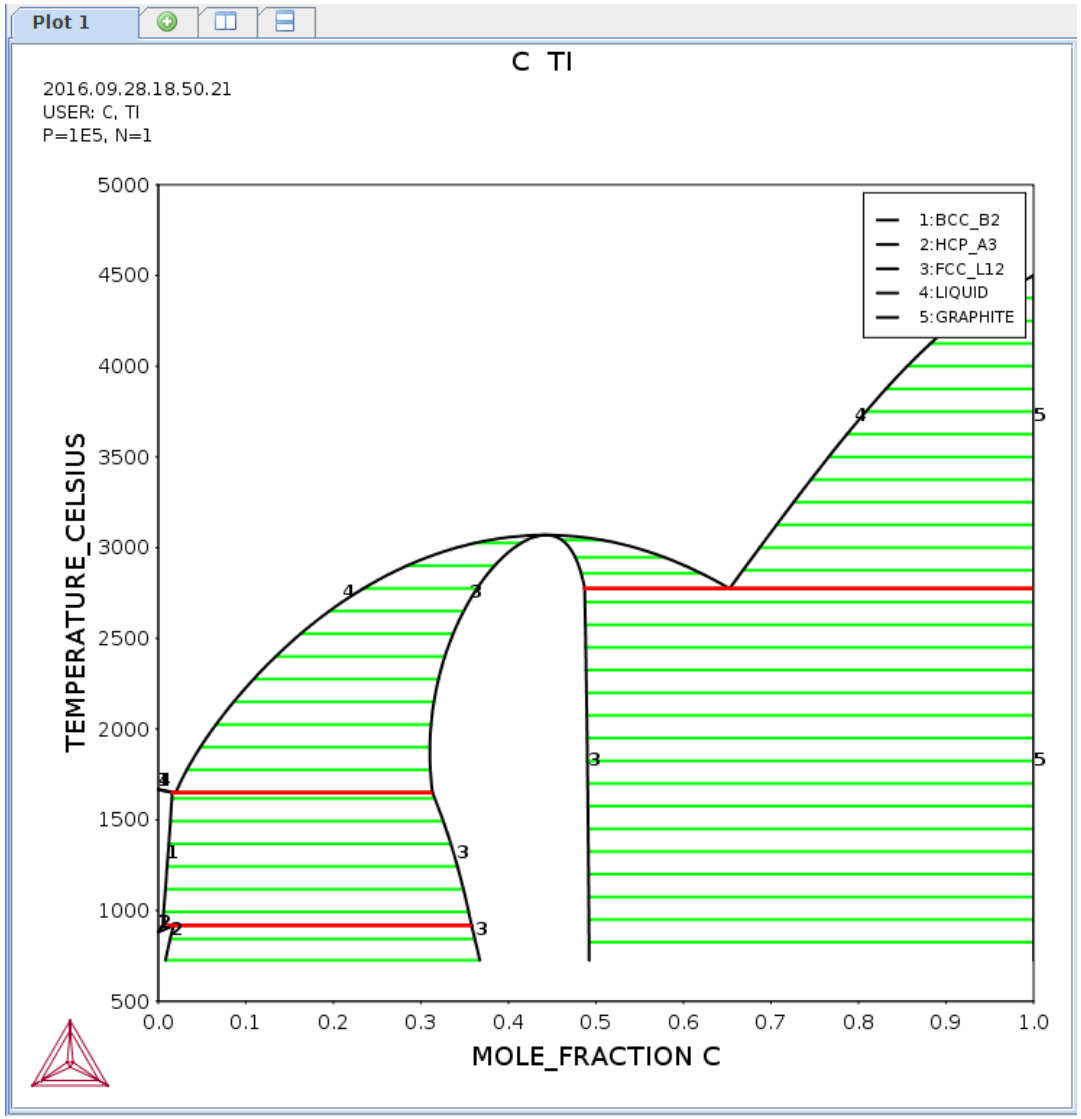
fcc ordering

```
POST:
POST:change_legend
SET SUFFIX FOR PHASE NAMES IN LEGEND? (ALL,NONE,CONSTITUTION,ORDERING) /NONE/:ordering
```



MC

```
go bin
TCNI
Ti C
```



MC

```
go bin
TCNI
Ti C


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

N
```

```
Output from POLY-3, equilibrium =     1, label A0  , 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  1.00000E+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 3.3532E+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  1.00000E+00
Sublattice  2,  Number of sites  2.5000E-01
TI  1.00000E+00
Sublattice  3,  Number of sites  1.0000E+00
C   6.66667E-01  VA  3.33333E-01
```

MC

```
go bin
TCNI
Ti C


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

N
```

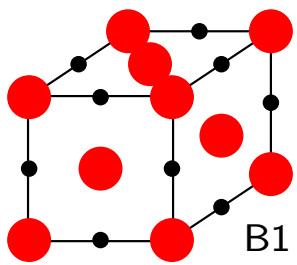
```
Output from POLY-3, equilibrium =     1, label A0  , database: USER

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  1.00000E+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 3.3532E+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
```



MC

```
go bin
TCNI
Ti C


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

N
```

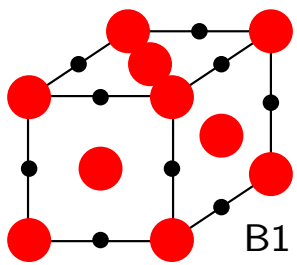
```
Output from POLY-3, equilibrium =     1, label A0  , database: USER

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  1.00000E+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 3.3532E+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  1.00000E+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                      8.4000E-01  8.8737E-01 2.1343E-03 -6.1357E+04 SER
TI                      1.0000E-01  8.6182E-02 8.6404E-09 -1.8525E+05 SER

FCC_L12#2                DISORD Status ENTERED   Driving force  0.0000E+00
Moles 6.4369E-01, Mass 3.6583E+01, Volume fraction 6.3940E-01  Mass fractions:
NI  9.19275E-01  TI  6.64621E-02  AL  1.39315E-02  C   3.31681E-04
Constitution:
Sublattice  1,  Number of sites  7.5000E-01
NI  8.91595E-01  TI  7.90144E-02  AL  2.93907E-02
Sublattice  2,  Number of sites  2.5000E-01
NI  8.91595E-01  TI  7.90144E-02  AL  2.93907E-02
Sublattice  3,  Number of sites  1.0000E+00
VA  9.98428E-01  C   1.57191E-03

FCC_L12#3                ORD    Status ENTERED   Driving force  0.0000E+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  7.5000E-01
NI  9.99873E-01  AL  8.02817E-05  TI  4.69657E-05
Sublattice  2,  Number of sites  2.5000E-01
TI  4.79911E-01  AL  3.67115E-01  NI  1.52974E-01
Sublattice  3,  Number of sites  1.0000E+00
VA  9.97117E-01  C   2.88321E-03

FCC_L12                  DISORD Status ENTERED   Driving force  0.0000E+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  7.5000E-01
TI  9.99882E-01  NI  1.17698E-04  AL  2.55338E-11
Sublattice  2,  Number of sites  2.5000E-01
TI  9.99882E-01  NI  1.17698E-04  AL  2.55338E-11
Sublattice  3,  Number of sites  1.0000E+00
C   9.35573E-01  VA  6.44271E-02
```

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
```

The FCC_L12 phase describes

- γ, A1
- γ', $L1_2$
- MC, B1.

```
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  1.00000E+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                      8.4000E-01  8.8737E-01 2.1343E-03 -6.1357E+04 SER
TI                      1.0000E-01  8.6182E-02 8.6404E-09 -1.8525E+05 SER

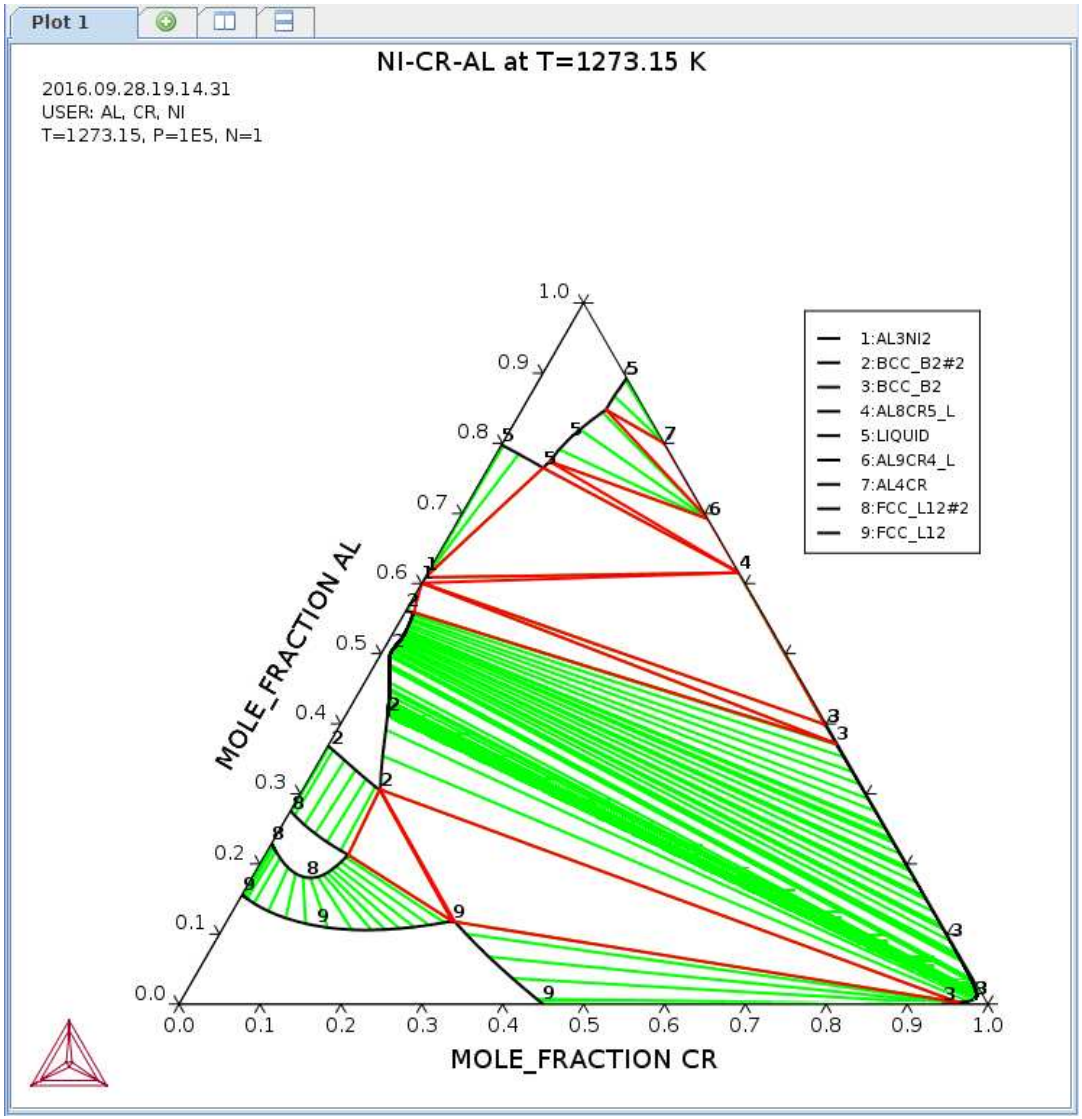
FCC_L12#2                DISORD Status ENTERED   Driving force  0.0000E+00
Moles 6.4369E-01, Mass 3.6583E+01, Volume fraction 6.3940E-01  Mass fractions:
NI  9.19275E-01  TI  6.64621E-02  AL  1.39315E-02  C   3.31681E-04
Constitution:
Sublattice  1,  Number of sites  7.5000E-01
NI  8.91595E-01  TI  7.90144E-02  AL  2.93907E-02
Sublattice  2,  Number of sites  2.5000E-01
NI  8.91595E-01  TI  7.90144E-02  AL  2.93907E-02
Sublattice  3,  Number of sites  1.0000E+00
VA  9.98428E-01  C   1.57191E-03

FCC_L12#3                ORD    Status ENTERED   Driving force  0.0000E+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  7.5000E-01
NI  9.99873E-01  AL  8.02817E-05  TI  4.69657E-05
Sublattice  2,  Number of sites  2.5000E-01
TI  4.79911E-01  AL  3.67115E-01  NI  1.52974E-01
Sublattice  3,  Number of sites  1.0000E+00
VA  9.97117E-01  C   2.88321E-03

FCC_L12                  DISORD Status ENTERED   Driving force  0.0000E+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  7.5000E-01
TI  9.99882E-01  NI  1.17698E-04  AL  2.55338E-11
Sublattice  2,  Number of sites  2.5000E-01
TI  9.99882E-01  NI  1.17698E-04  AL  2.55338E-11
Sublattice  3,  Number of sites  1.0000E+00
C   9.35573E-01  VA  6.44271E-02
```

bcc ordering

```
go ter
TCNI
Ni Cr Al
```



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

N
```

```
Conditions:
T=1273.15, P=1E5, N=1, X(CR)=0.1, X(NI)=0.5
DEGREES OF FREEDOM 0

Temperature   1273.15 K (  1000.00 C),  Pressure  1.000000E+05
Number of moles of components  1.00000E+00,  Mass in grams  4.53374E+01
Total Gibbs energy -1.09100E+05,  Enthalpy -2.39238E+04,  Volume  7.51285E-06

Component               Moles       W-Fraction  Activity   Potential  Ref.stat
AL                      4.0000E-01  2.3806E-01 8.9482E-07 -1.4742E+05 SER
CR                      1.0000E-01  1.1469E-01 6.4766E-03 -5.3347E+04 SER
NI                      5.0000E-01  6.4726E-01 2.1100E-04 -8.9593E+04 SER

BCC_B2#2                 ORD    Status ENTERED   Driving force  0.0000E+00
Moles 9.4336E-01, Mass 4.2403E+01, Volume fraction 9.4381E-01  Mass fractions:
NI  6.91280E-01  AL  2.54176E-01  CR  5.45440E-02
Constitution:
Sublattice  1,  Number of sites  5.0000E-01
NI  9.93291E-01  CR  6.21984E-03  VA  4.71098E-04  AL  1.85227E-05
Sublattice  2,  Number of sites  5.0000E-01
AL  8.46630E-01  CR  8.80601E-02  NI  6.53098E-02  VA  2.43856E-12
Sublattice  3,  Number of sites  3.0000E+00
VA  1.00000E+00

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:
CR  9.83643E-01  NI  1.12237E-02  AL  5.13316E-03
Constitution:
Sublattice  1,  Number of sites  5.0000E-01
CR  9.80233E-01  NI  9.90905E-03  AL  9.85763E-03  VA  1.06573E-09
Sublattice  2,  Number of sites  5.0000E-01
CR  9.80233E-01  NI  9.90905E-03  AL  9.85763E-03  VA  1.06573E-09
Sublattice  3,  Number of sites  3.0000E+00
VA  1.00000E+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

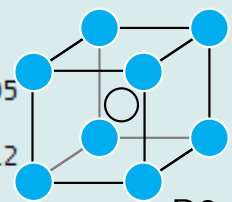
N
```

```
Conditions:
T=1273.15, P=1E5, N=1, X(CR)=0.1, X(NI)=0.5
DEGREES OF FREEDOM 0

Temperature   1273.15 K (  1000.00 C),  Pressure  1.000000E+05
Number of moles of components  1.00000E+00,  Mass in grams  4.53374E+01
Total Gibbs energy -1.09100E+05,  Enthalpy -2.39238E+04,  Volume  7.51285E-06

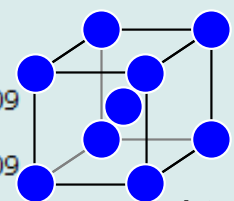
Component               Moles       W-Fraction  Activity   Potential  Ref.stat
AL                      4.0000E-01  2.3806E-01 8.9482E-07 -1.4742E+05 SER
CR                      1.0000E-01  1.1469E-01 6.4766E-03 -5.3347E+04 SER
NI                      5.0000E-01  6.4726E-01 2.1100E-04 -8.9593E+04 SER

BCC_B2#2                 ORD    Status ENTERED   Driving force  0.0000E+00
Moles 9.4336E-01, Mass 4.2403E+01, Volume fraction 9.4381E-01  Mass fractions:
NI  6.91280E-01  AL  2.54176E-01  CR  5.45440E-02
Constitution:
Sublattice  1,  Number of sites  5.0000E-01
NI  9.93291E-01  CR  6.21984E-03  VA  4.71098E-04  AL  1.85227E-05
Sublattice  2,  Number of sites  5.0000E-01
AL  8.46630E-01  CR  8.80601E-02  NI  6.53098E-02  VA  2.43856E-12
Sublattice  3,  Number of sites  3.0000E+00
VA  1.00000E+00
```



B2

```
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:
CR  9.83643E-01  NI  1.12237E-02  AL  5.13316E-03
Constitution:
Sublattice  1,  Number of sites  5.0000E-01
CR  9.80233E-01  NI  9.90905E-03  AL  9.85763E-03  VA  1.06573E-09
Sublattice  2,  Number of sites  5.0000E-01
CR  9.80233E-01  NI  9.90905E-03  AL  9.85763E-03  VA  1.06573E-09
Sublattice  3,  Number of sites  3.0000E+00
VA  1.00000E+00
```



A2

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

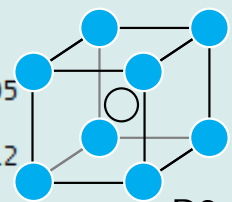
N
```

```
Conditions:
T=1273.15, P=1E5, N=1, X(CR)=0.1, X(NI)=0.5
DEGREES OF FREEDOM 0

Temperature   1273.15 K (  1000.00 C),  Pressure  1.000000E+05
Number of moles of components  1.00000E+00,  Mass in grams  4.53374E+01
Total Gibbs energy -1.09100E+05,  Enthalpy -2.39238E+04,  Volume  7.51285E-06

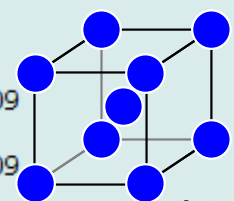
Component               Moles       W-Fraction  Activity   Potential  Ref.stat
AL                      4.0000E-01  2.3806E-01 8.9482E-07 -1.4742E+05 SER
CR                      1.0000E-01  1.1469E-01 6.4766E-03 -5.3347E+04 SER
NI                      5.0000E-01  6.4726E-01 2.1100E-04 -8.9593E+04 SER

BCC_B2#2                 ORD    Status ENTERED   Driving force  0.0000E+00
Moles 9.4336E-01, Mass 4.2403E+01, Volume fraction 9.4381E-01  Mass fractions:
NI  6.91280E-01  AL  2.54176E-01  CR  5.45440E-02
Constitution:
Sublattice  1,  Number of sites  5.0000E-01
NI  9.93291E-01  CR  6.21984E-03  VA  4.71098E-04  AL  1.85227E-05
Sublattice  2,  Number of sites  5.0000E-01
AL  8.46630E-01  CR  8.80601E-02  NI  6.53098E-02  VA  2.43856E-12
Sublattice  3,  Number of sites  3.0000E+00
VA  1.00000E+00
```



B2

```
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:
CR  9.83643E-01  NI  1.12237E-02  AL  5.13316E-03
Constitution:
Sublattice  1,  Number of sites  5.0000E-01
CR  9.80233E-01  NI  9.90905E-03  AL  9.85763E-03  VA  1.06573E-09
Sublattice  2,  Number of sites  5.0000E-01
CR  9.80233E-01  NI  9.90905E-03  AL  9.85763E-03  VA  1.06573E-09
Sublattice  3,  Number of sites  3.0000E+00
VA  1.00000E+00
```



A2

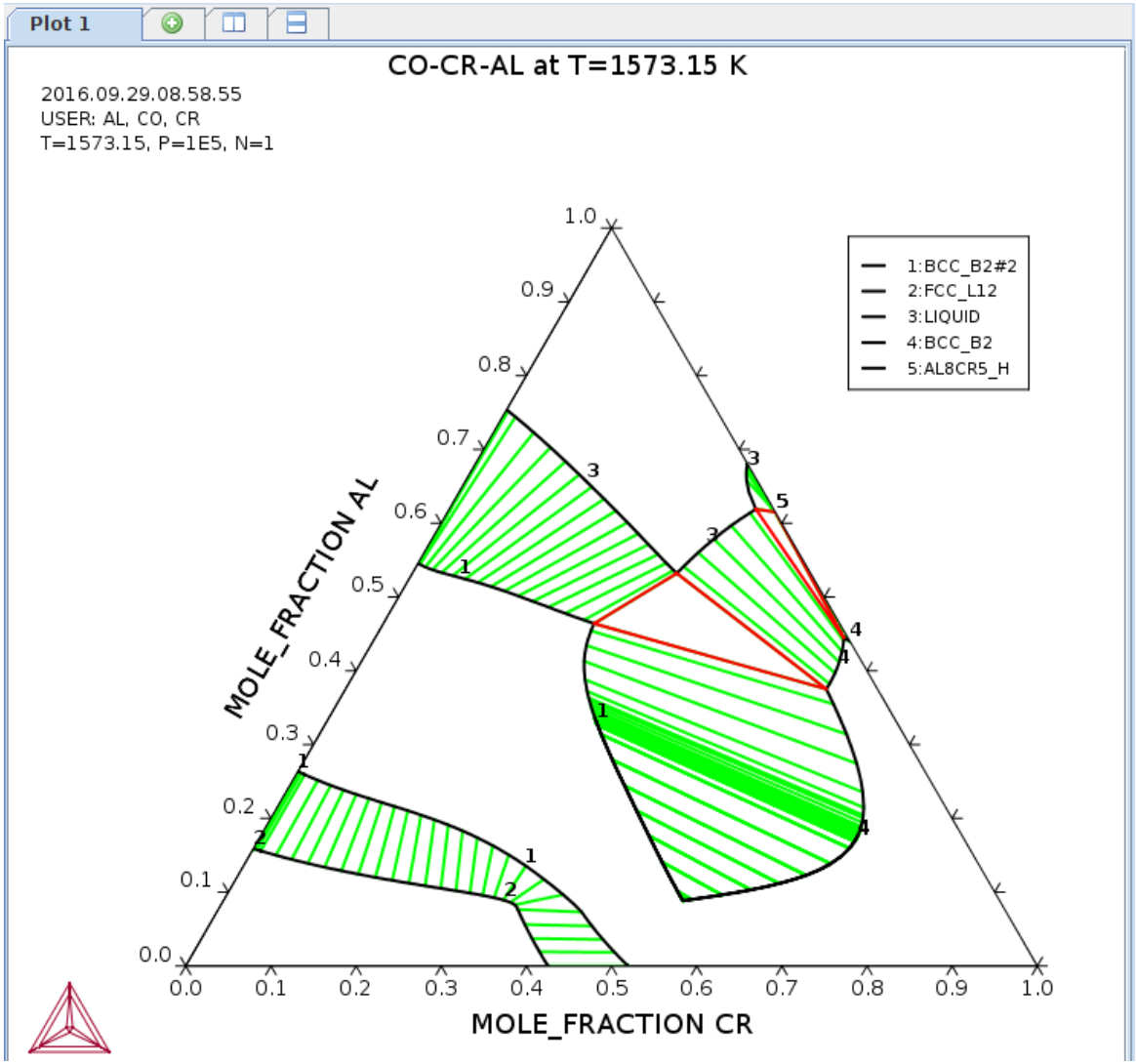
The BCC_B2 phase describes

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

2nd order transition

```
go ter
TCNI
Co Cr Al

1300
```



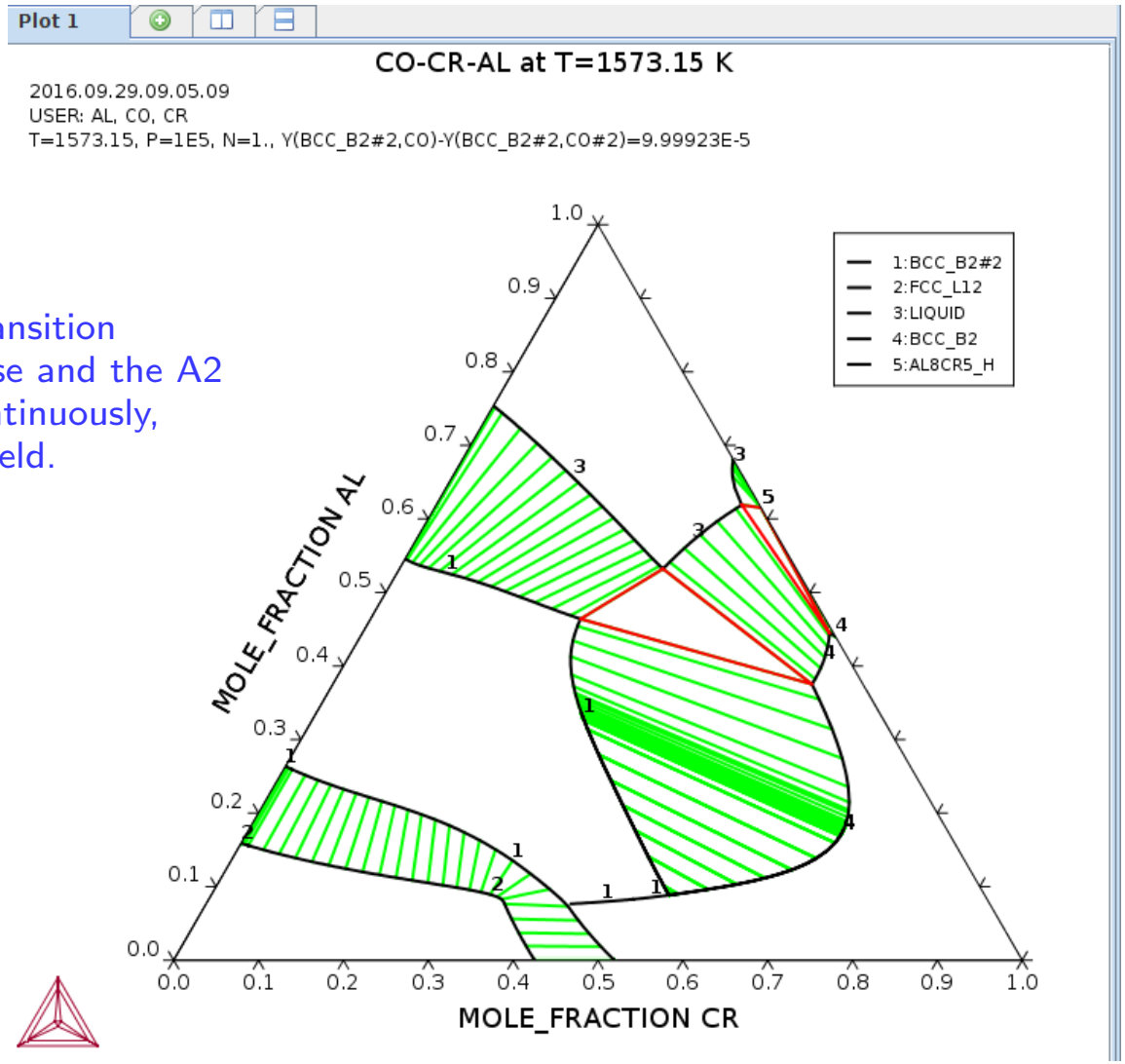
2nd order transition

```
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 ccontinuously, without A2+B2 two phase field.



2nd order transition

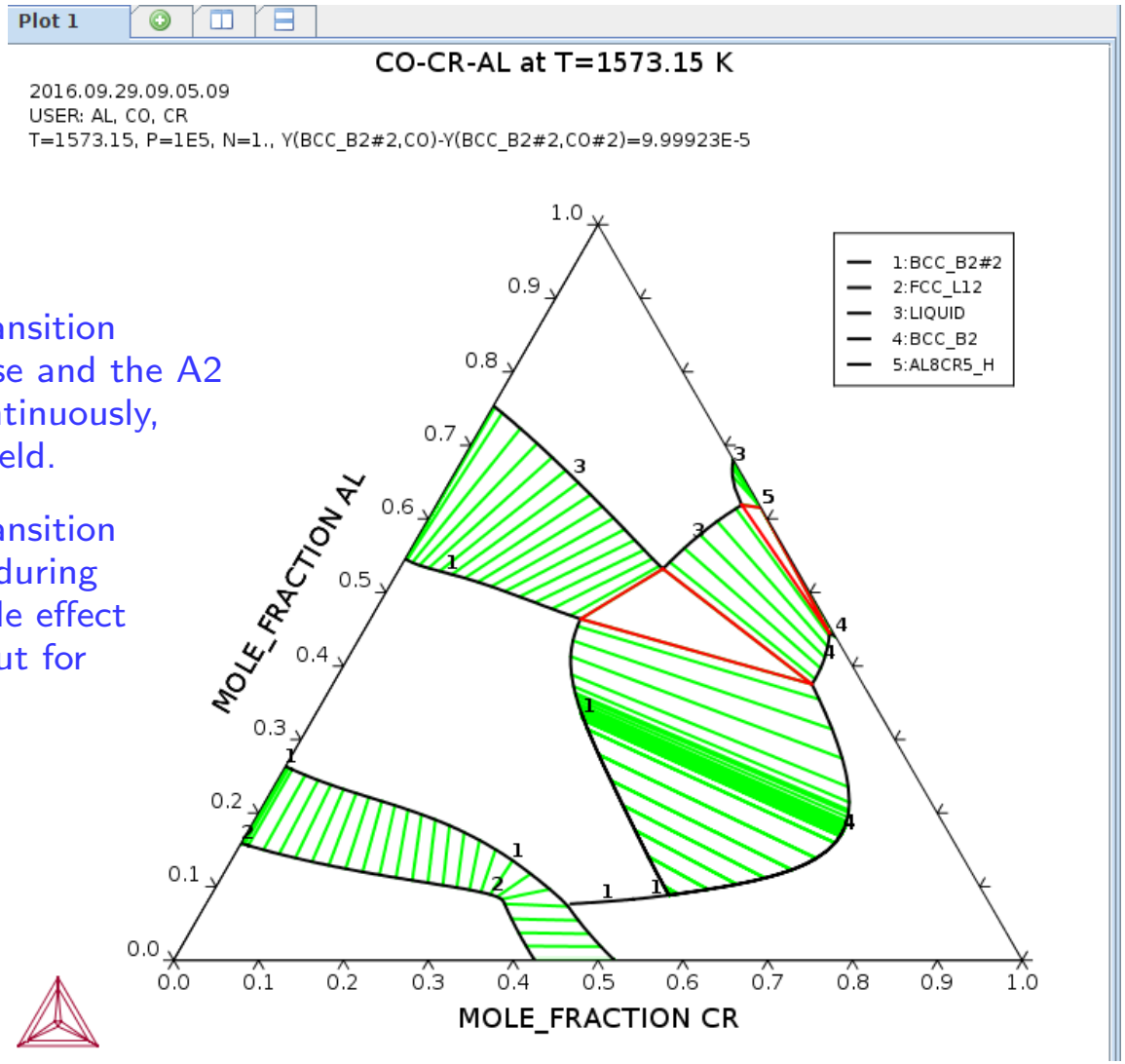
```
go ter
TCNI
Co Cr Al

1300

...
```

There is a field where the transition between the B2 ordered phase and the A2 disordered phase occurs ccontinuously, 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.



2nd order transition

```
go ter
TCNI
Co Cr Al

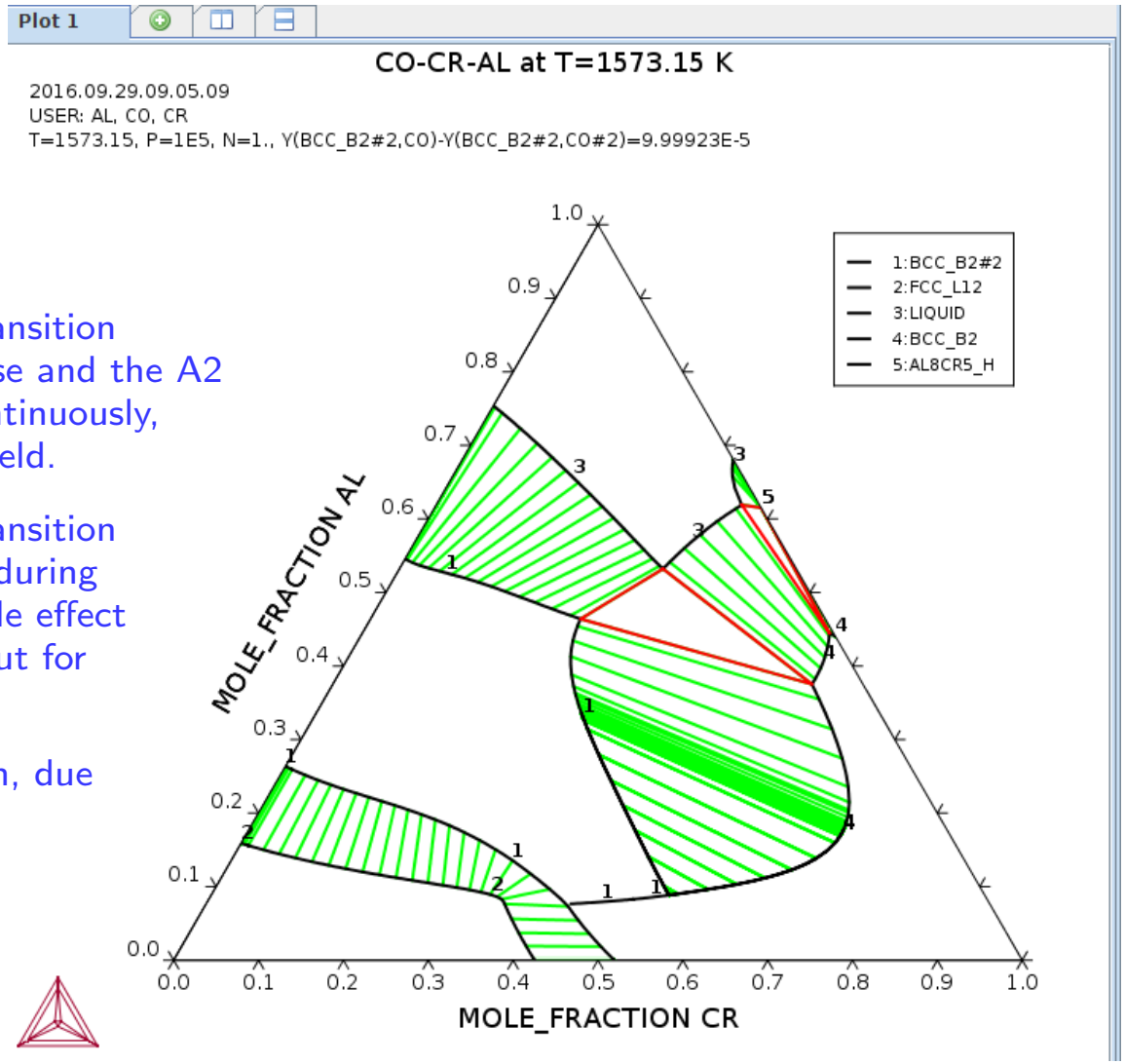
1300

...
```

There is a field where the transition between the B2 ordered phase and the A2 disordered phase occurs ccontinuously, 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 λ transition, due to the shape of the Cp curve during such a transition.



2nd order transition

```
go ter
TCNI
Co Cr Al

1300

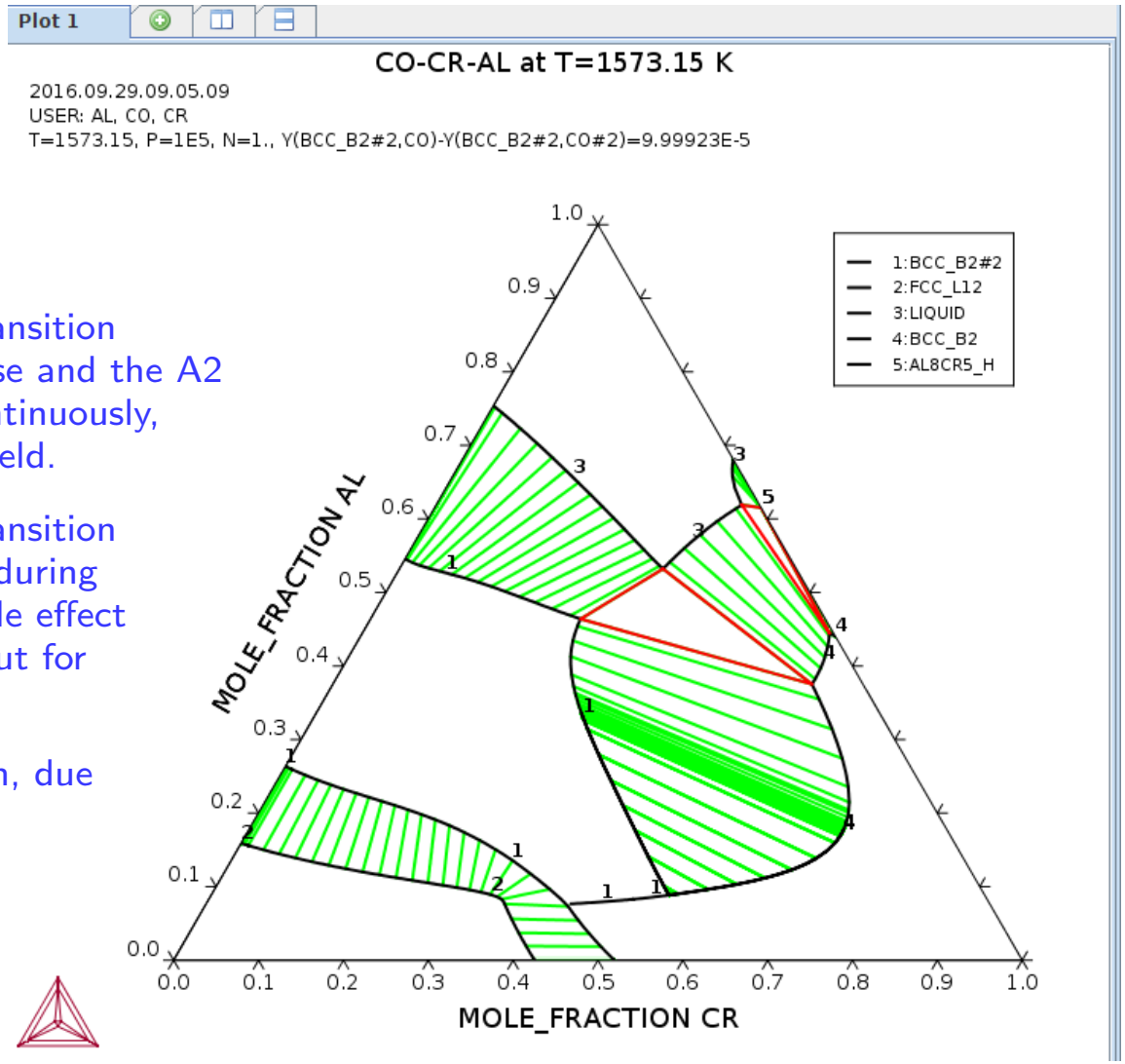
...
```

There is a field where the transition between the B2 ordered phase and the A2 disordered phase occurs ccontinuously, 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 λ 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 charaterized 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/$L1_2$ and A2/B2, allowing in particular to describe the second order transition of these latter.