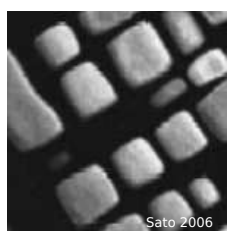
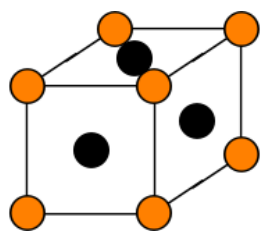
The TCNI database

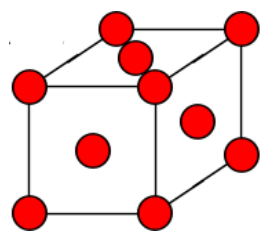
Nathalie Dupin

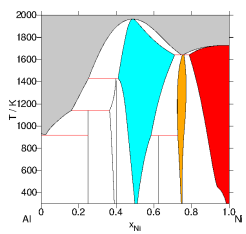
Calcul Thermodynamique

Paris, Ecole des Mines, 20 oct. 2016







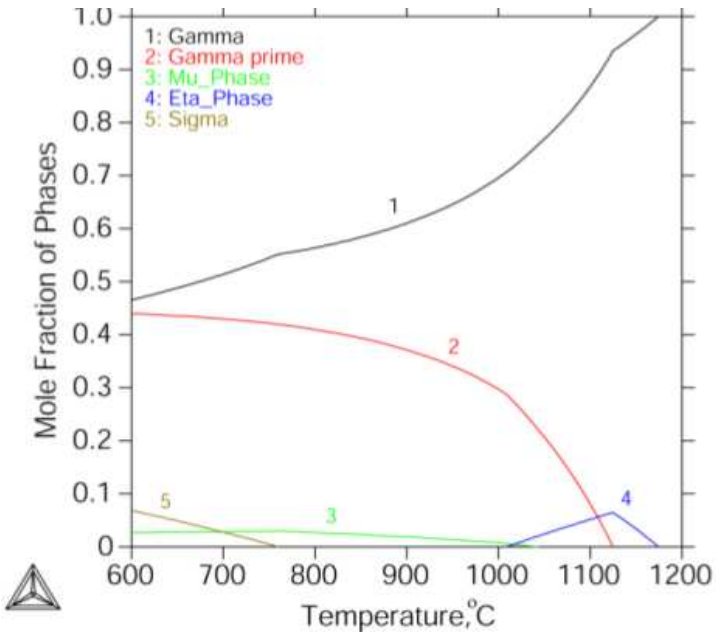


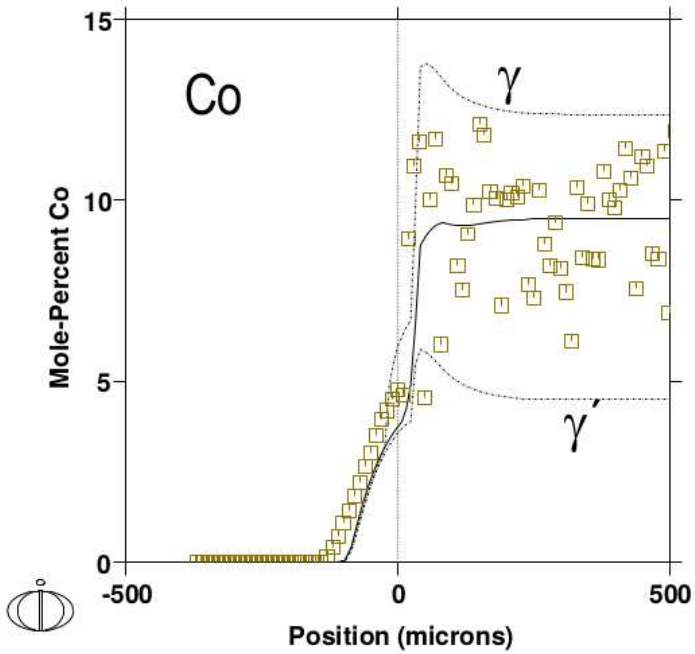
Plan

- Généralités
- fcc
  - Mise en ordre
  - MC
- cc
  - Mise en ordre
  - 2nd ordre
- Conclusion

TCNI

- Base de données thermodynamiques commerciale développée par TCSAB dans le cadre d'une collaboration avec des partenaires industriels pour décrire les équilibres de phases dans les superalliages.

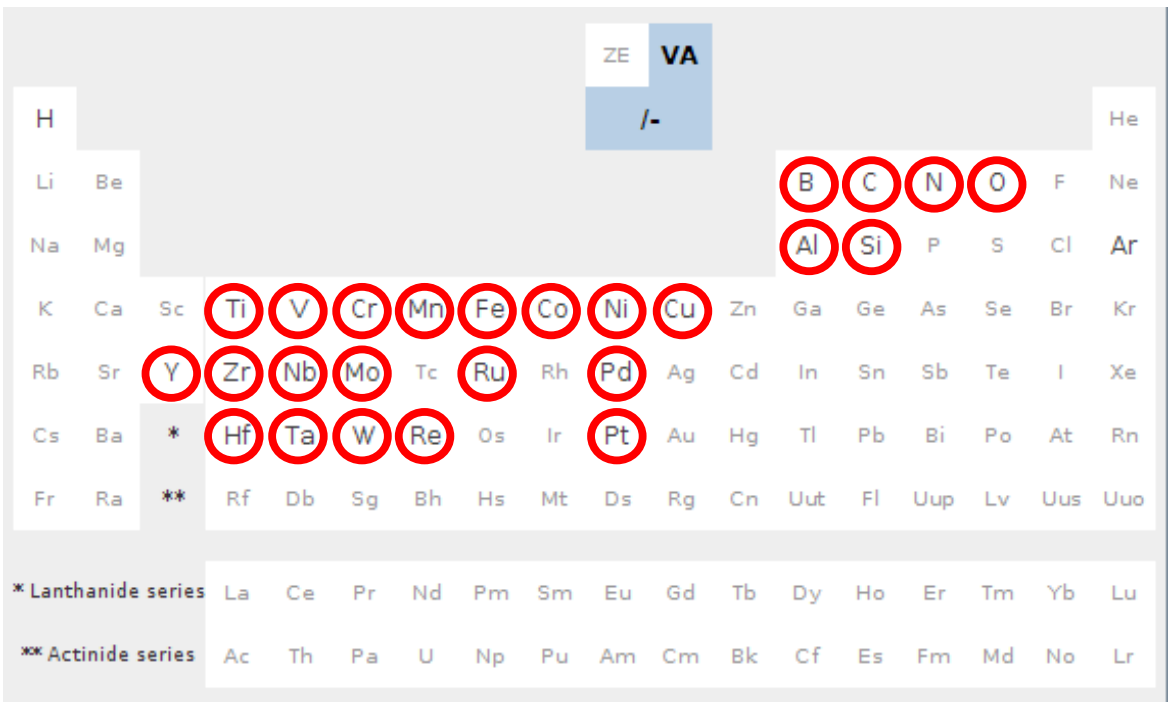




J. Bratberg *et al.* Superalloys 2012

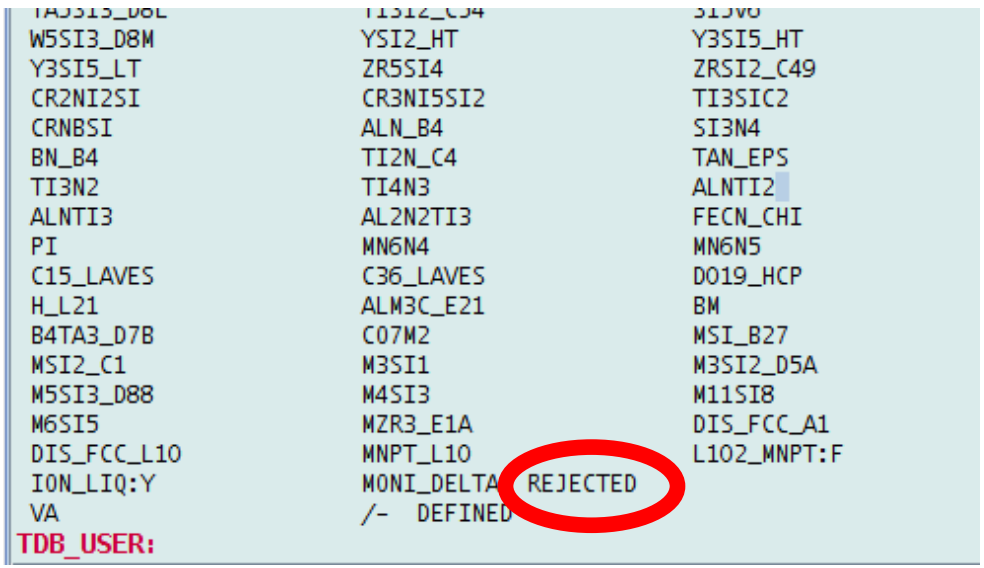
TCNI

- Base de données thermodynamiques commerciale développée par TCSAB dans le cadre d'une collaboration avec des partenaires industriels pour décrire les équilibres de phases dans les superalliages.
- Tous les binaires du système complexe Al-B-C-Co-Cr-Fe-Hf-Mn-Mo-N-Nb-Ni-O-Pd-Pt-Re-Ru-Si-Ta-Ti-V-W-Y-Zr sont décrits.



TCNI

- Base de données thermodynamiques commerciale développée par TCSAB dans le cadre d'une collaboration avec des partenaires industriels pour décrire les équilibres de phases dans les superalliages.
- Tous les binaires du système complexe Al-B-C-Co-Cr-Fe-Hf-Mn-Mo-N-Nb-Ni-O-Pd-Pt-Re-Ru-Si-Ta-Ti-V-W-Y-Zr sont décrits.
- Seules les phases d'intérêt pour les alliages industriels sont extraites par défaut.



Lorsque la base est sélectionnée, la liste de toutes les phases rejetée par défaut apparaît.

L'utilisateur peut évidemment restaurer les phases qu'il considère nécessaires pour un calcul spécifique.

TCNI

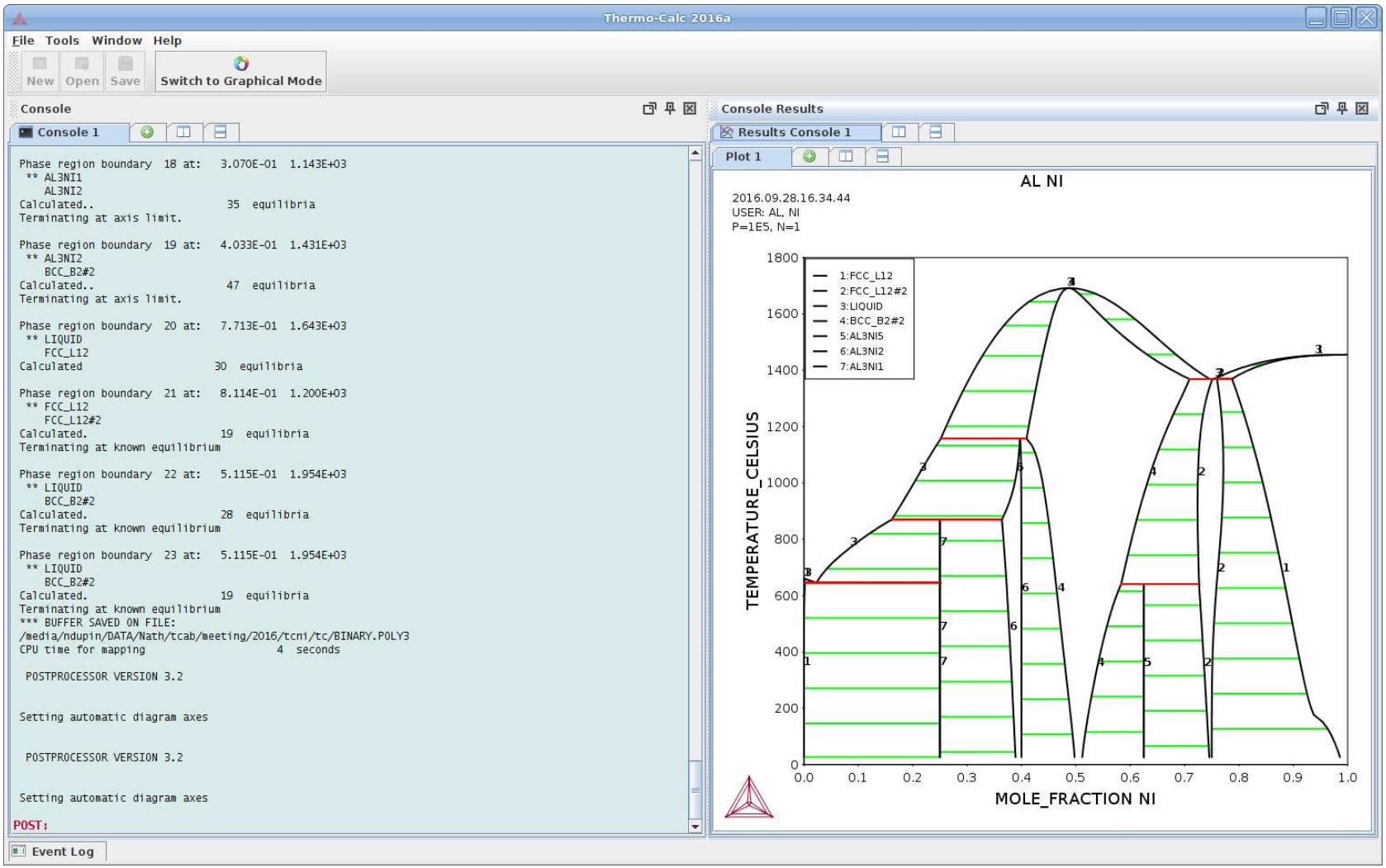
- Base de données thermodynamiques commerciale développée par TCSAB dans le cadre d'une collaboration avec des partenaires industriels pour décrire les équilibres de phases dans les superalliages.
- Tous les binaires du système complexe Al-B-C-Co-Cr-Fe-Hf-Mn-Mo-N-Nb-Ni-O-Pd-Pt-Re-Ru-Si-Ta-Ti-V-W-Y-Zr sont décrits.
- Seules les phases d'intérêt pour les alliages industriels sont extraites par défaut.
- Les descriptions complètes des systèmes binaires et des systèmes ternaires évalués sont accessibles en utilisant les modules `BINARY` et `TERNARY`.

TCNI

- Base de données thermodynamiques commerciale développée par TCSAB dans le cadre d'une collaboration avec des partenaires industriels pour décrire les équilibres de phases dans les superalliages.
- Tous les binaires du système complexe Al-B-C-Co-Cr-Fe-Hf-Mn-Mo-N-Nb-Ni-O-Pd-Pt-Re-Ru-Si-Ta-Ti-V-W-Y-Zr sont décrits.
- Seules les phases d'intérêt pour les alliages industriels sont extraites par défaut.
- Les descriptions complètes des systèmes binaires et des systèmes ternaires évalués sont accessibles en utilisant les modules `BINARY` et `TERNARY`.
- Cette base de données se caractérise par l'utilisation d'une seule équation pour les phases $A1/L1_2$ d'une part et $A2/B2$ d'autre part qui présentent des relations crystallographiques d'ordre.

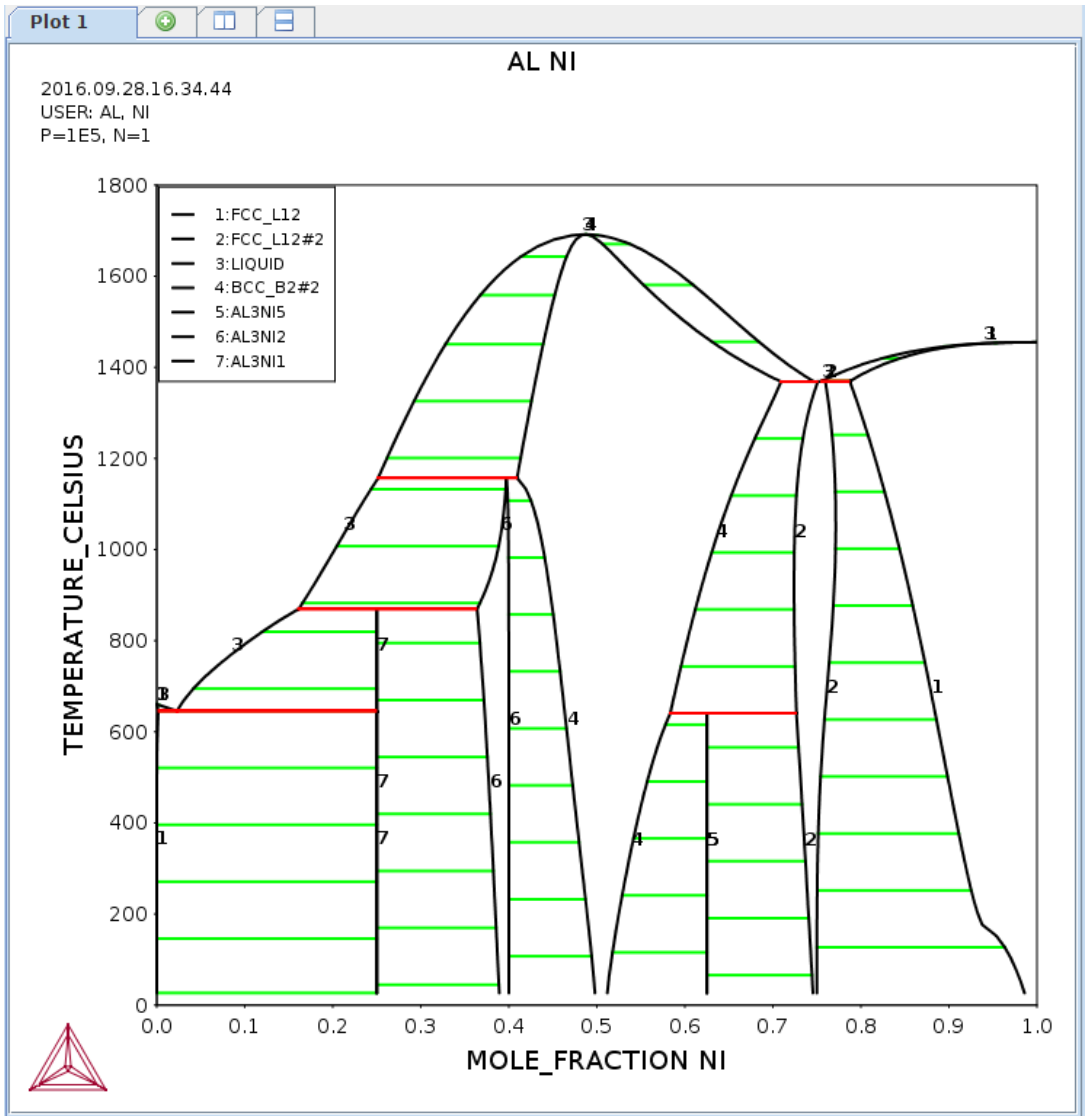
Mise en ordre fcc

```
go bin
TCNI
Al
Ni
```



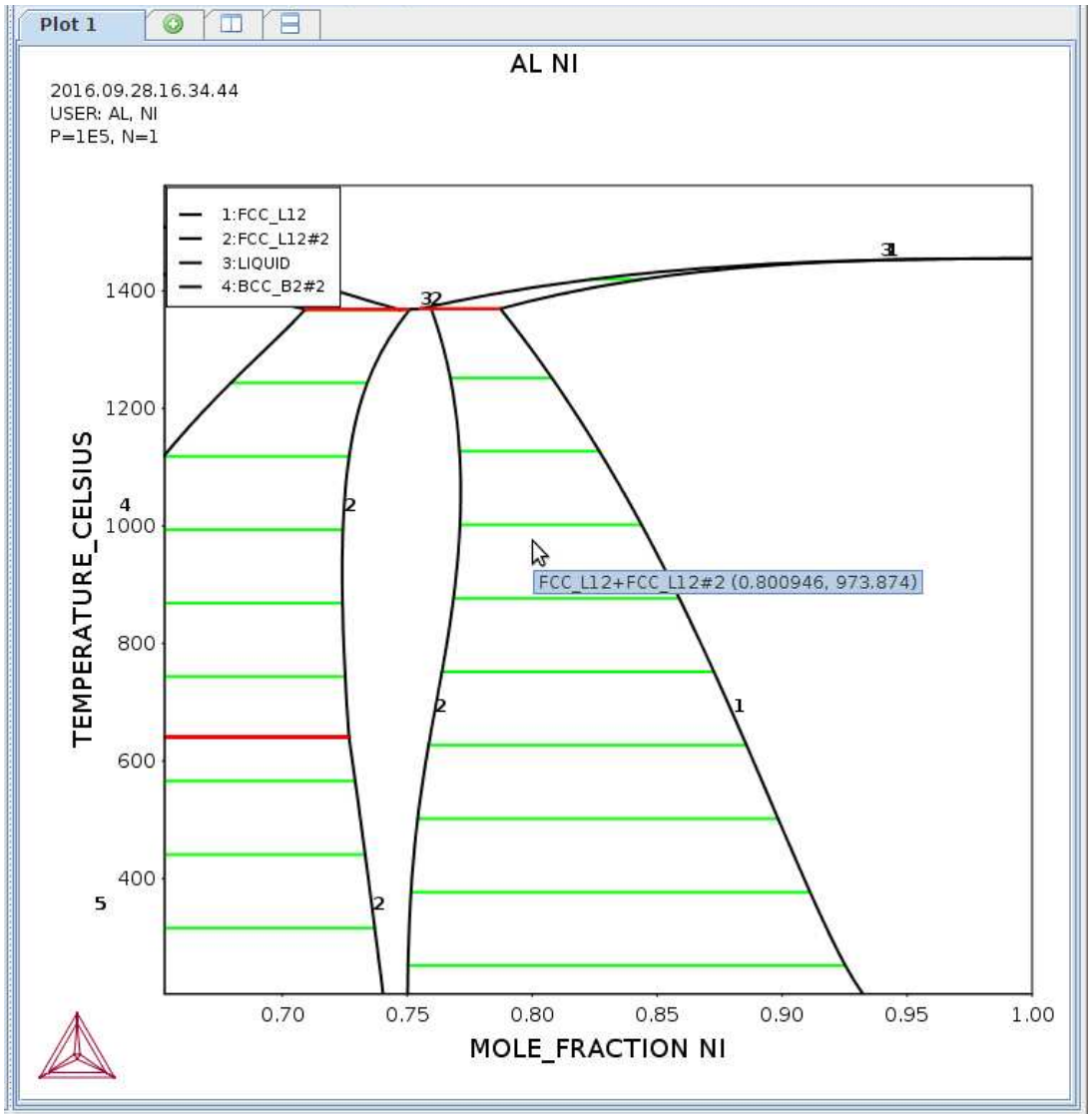
Mise en ordre fcc

```
go bin
TCNI
Al
Ni
```



Mise en ordre fcc

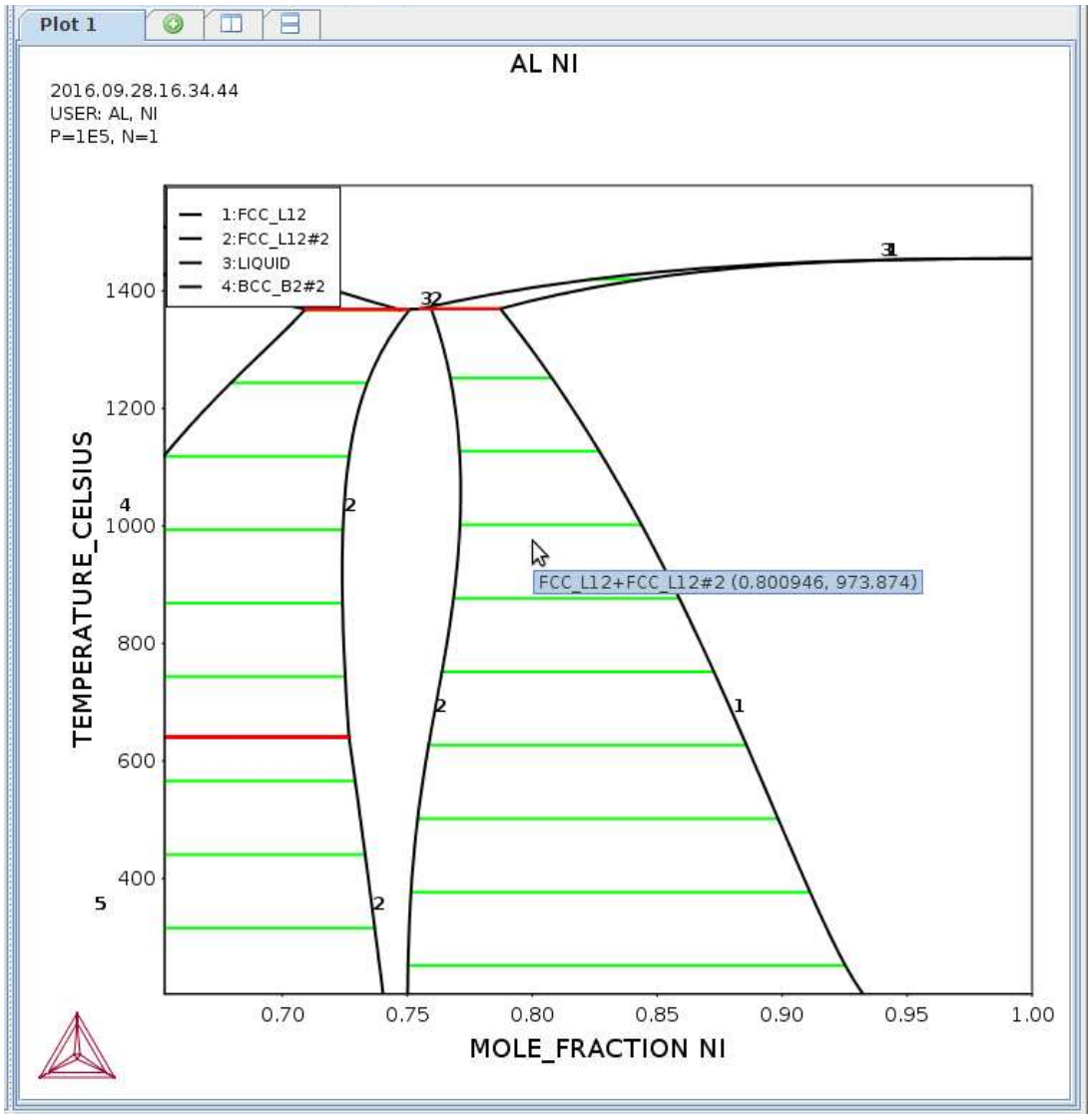
```
go bin
TCNI
Al
Ni
```



Mise en ordre fcc

```
go bin
TCNI
Al
Ni

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



Mise en ordre fcc

```
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
```

Mise en ordre fcc

```
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

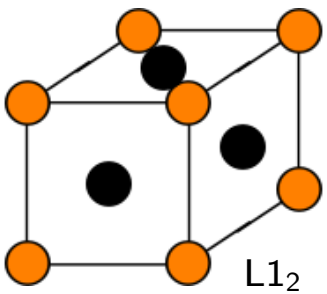
 FCC_L12#2               ORD    Status ENTERED   Driving force  0.0000E+00
 Moles 6.3732E-01, Mass 3.2754E+01, Volume fraction 6.4022E-01  Mass fractions:
 NI  8.79167E-01  AL  1.20833E-01
 Constitution:
 Sublattice  1,  Number of sites  7.5000E-01
 NI  9.95375E-01  AL  4.62502E-03
 Sublattice  2,  Number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

Mise en ordre fcc

```
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
```

Mise en ordre fcc

```
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

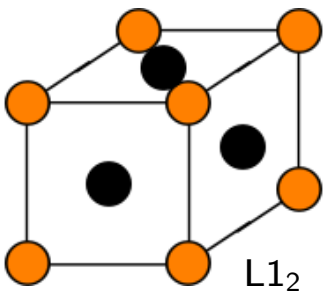
 Conditions:
 X(NI)=0.8, P=1E5, N=1, T=1200
 DEGREES OF FREEDOM 0

 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

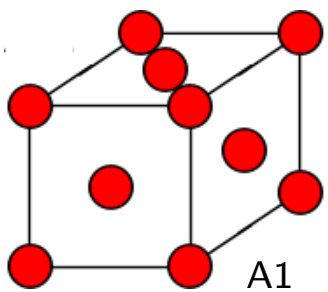
 Component              Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                     2.0000E-01  1.0309E-01 1.7170E-06 -1.3245E+05 FCC_A1
 NI                     8.0000E-01  8.9691E-01 6.8371E-01 -3.7936E+03 FCC_A1

 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

Mise en ordre fcc

```
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

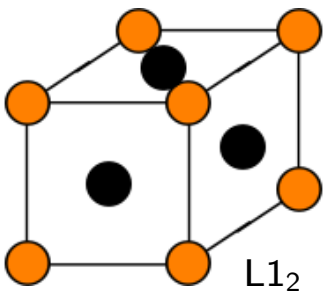
 Conditions:
 X(NI)=0.8, P=1E5, N=1, T=1200
 DEGREES OF FREEDOM 0

 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

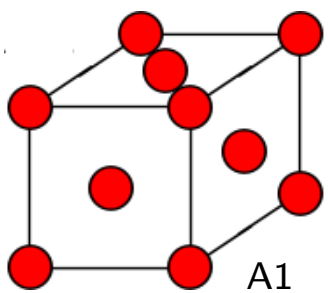
 FCC_L12                  DISORD Status ENTERED   Driving force  0.0000E+00
 Moles 3.6268E-01, Mass 1.9595E+01, Volume fraction 3.5978E-01  Mass fractions:
 NI  9.26579E-01  AL  7.34214E-02
 Constitution:
 Sublattice  1,  Number of sites  7.5000E-01
 NI  8.52982E-01  AL  1.47018E-01
 Sublattice  2,  Number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



$L1_2$

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

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



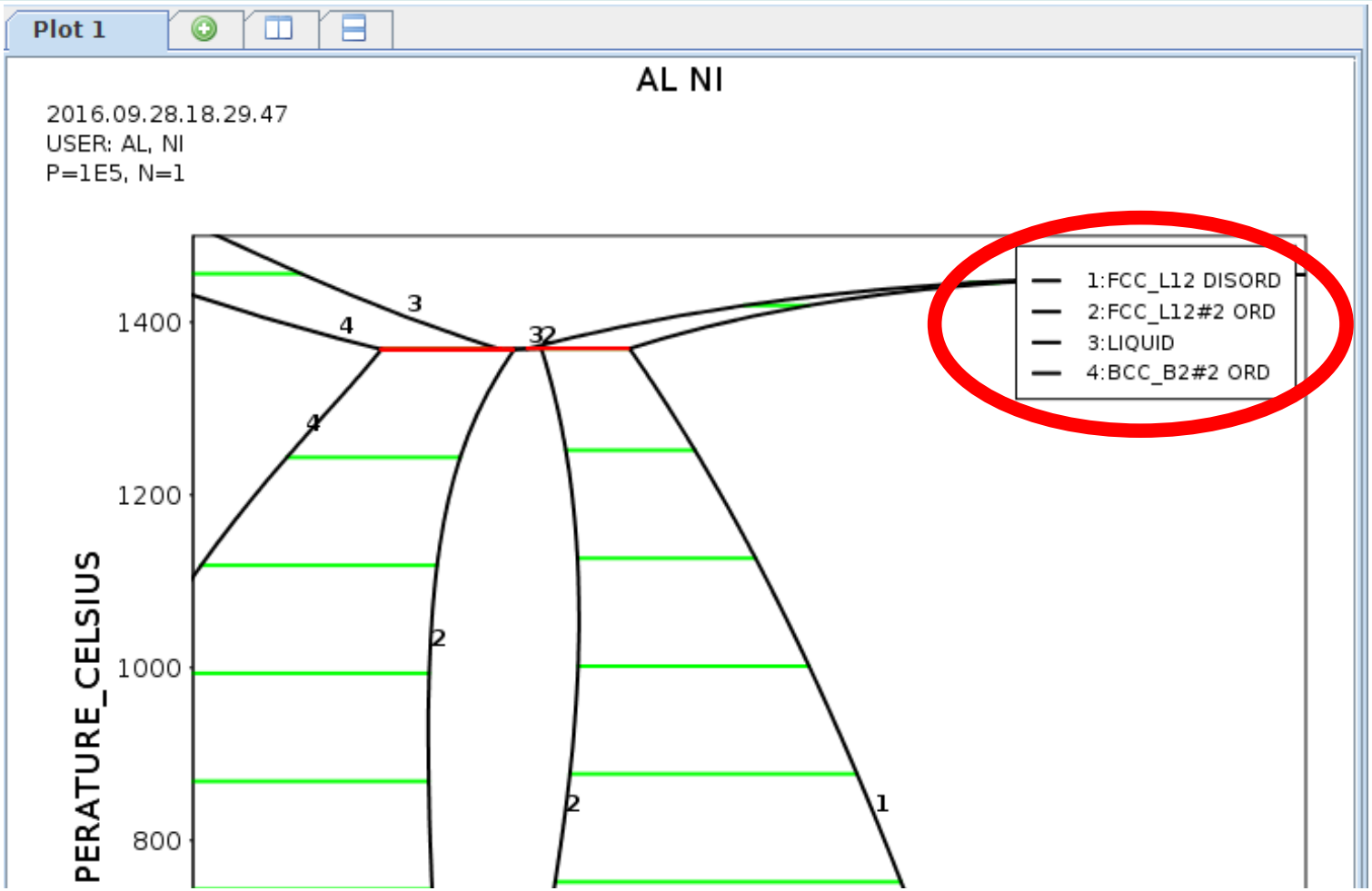
A1

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

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

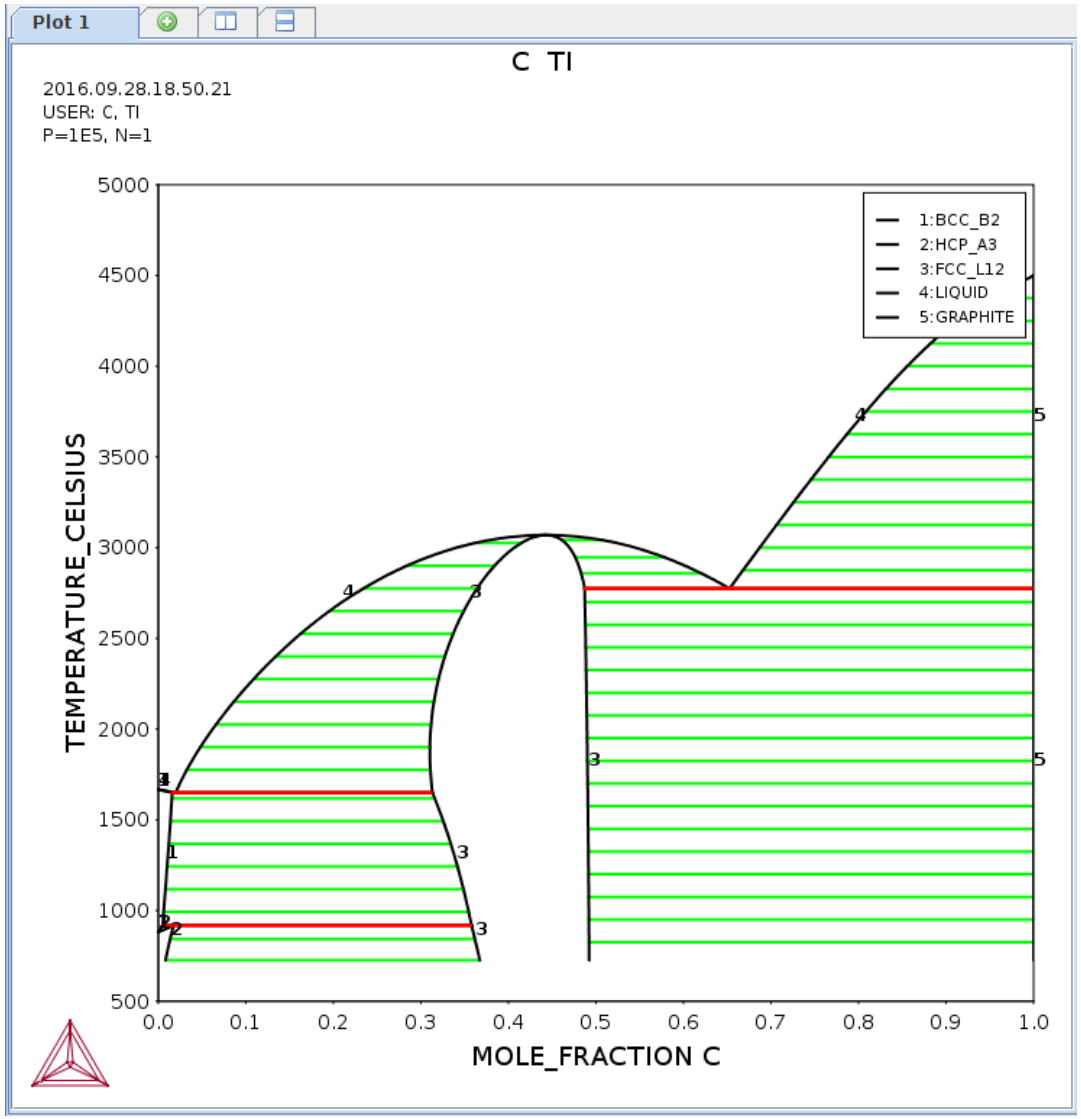
Mise en ordre fcc

```
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
```

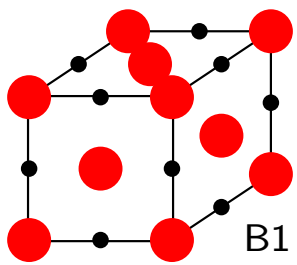
```
Output from POLY-3, equilibrium =     1, label A0  , database: USER

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
```

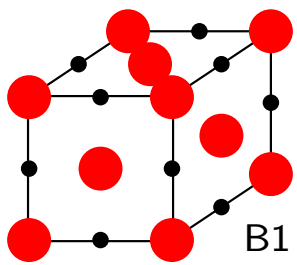
```
Output from POLY-3, equilibrium =     1, label A0  , database: USER

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
```



La phase FCC_L12 décrit également les carbures cubiques de type MC lorsque le dernier sous-réseau contient une fraction importante de 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
```

La phase FCC_L12 décrit

- 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

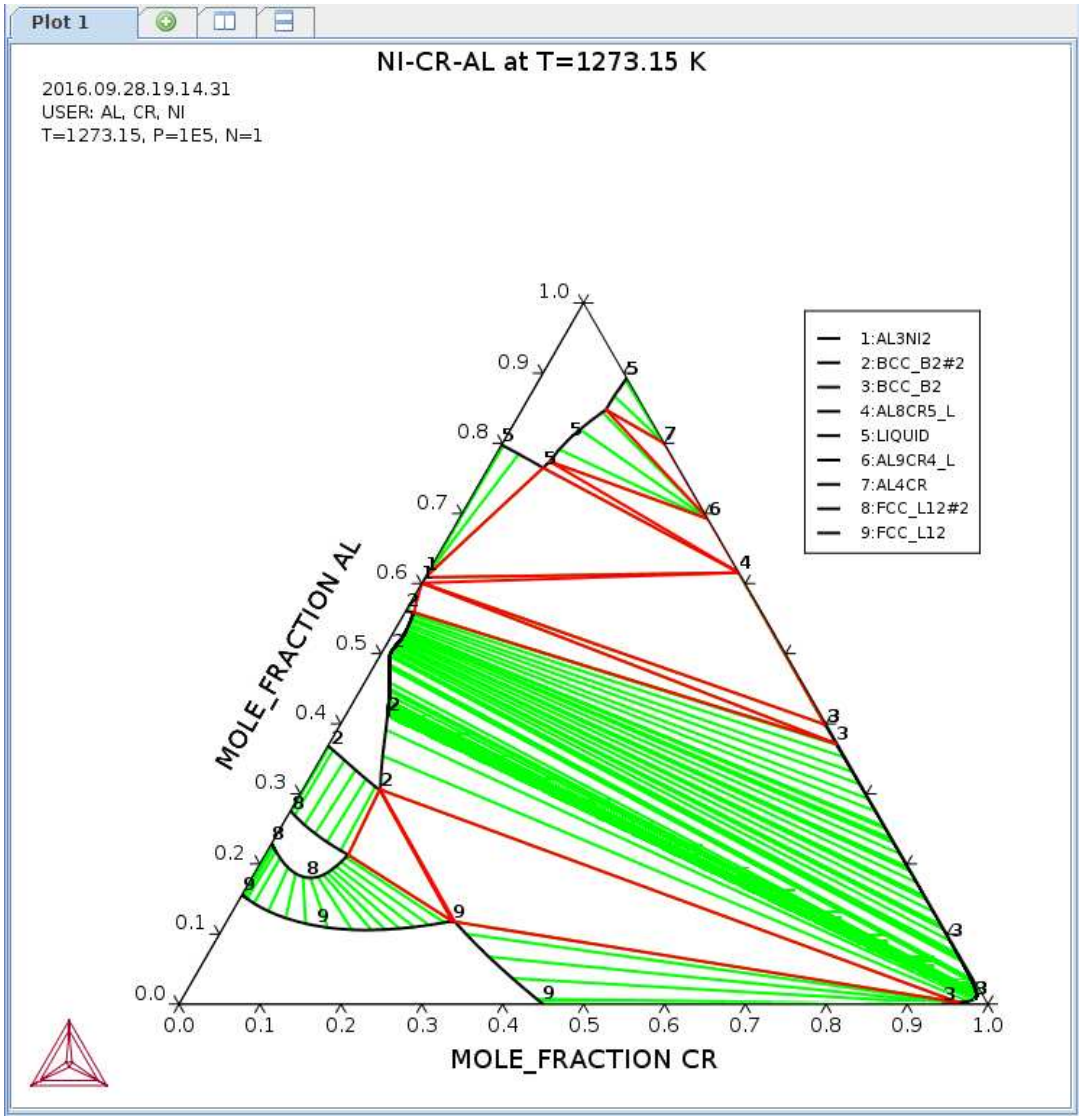
FCC_L12#2                DISORD Status ENTERED   Driving force  0.0000E+00
Moles 6.4369E-01, Mass 3.6583E+01, Volume fraction 6.3940E-01  Mass fractions:
NI  9.19275E-01  TI  6.64621E-02  AL  1.39315E-02  C   3.31681E-04
Constitution:
Sublattice  1,  Number of sites  7.5000E-01
NI  8.91595E-01  TI  7.90144E-02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

Mise en ordre cc

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



Mise en ordre cc

```
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
```

Mise en ordre cc

```
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

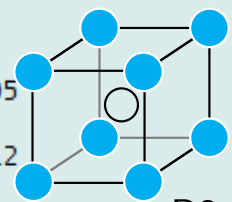
N
```

```
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

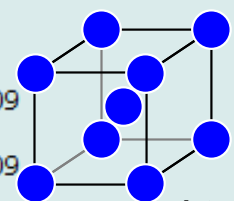
Component               Moles       W-Fraction  Activity   Potential  Ref.stat
AL                      4.0000E-01  2.3806E-01 8.9482E-07 -1.4742E+05 SER
CR                      1.0000E-01  1.1469E-01 6.4766E-03 -5.3347E+04 SER
NI                      5.0000E-01  6.4726E-01 2.1100E-04 -8.9593E+04 SER

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

Mise en ordre cc

```
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

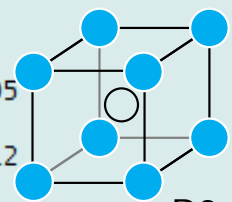
N
```

```
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

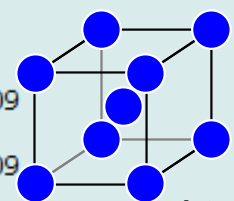
Component               Moles       W-Fraction  Activity   Potential  Ref.stat
AL                      4.0000E-01  2.3806E-01 8.9482E-07 -1.4742E+05 SER
CR                      1.0000E-01  1.1469E-01 6.4766E-03 -5.3347E+04 SER
NI                      5.0000E-01  6.4726E-01 2.1100E-04 -8.9593E+04 SER

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

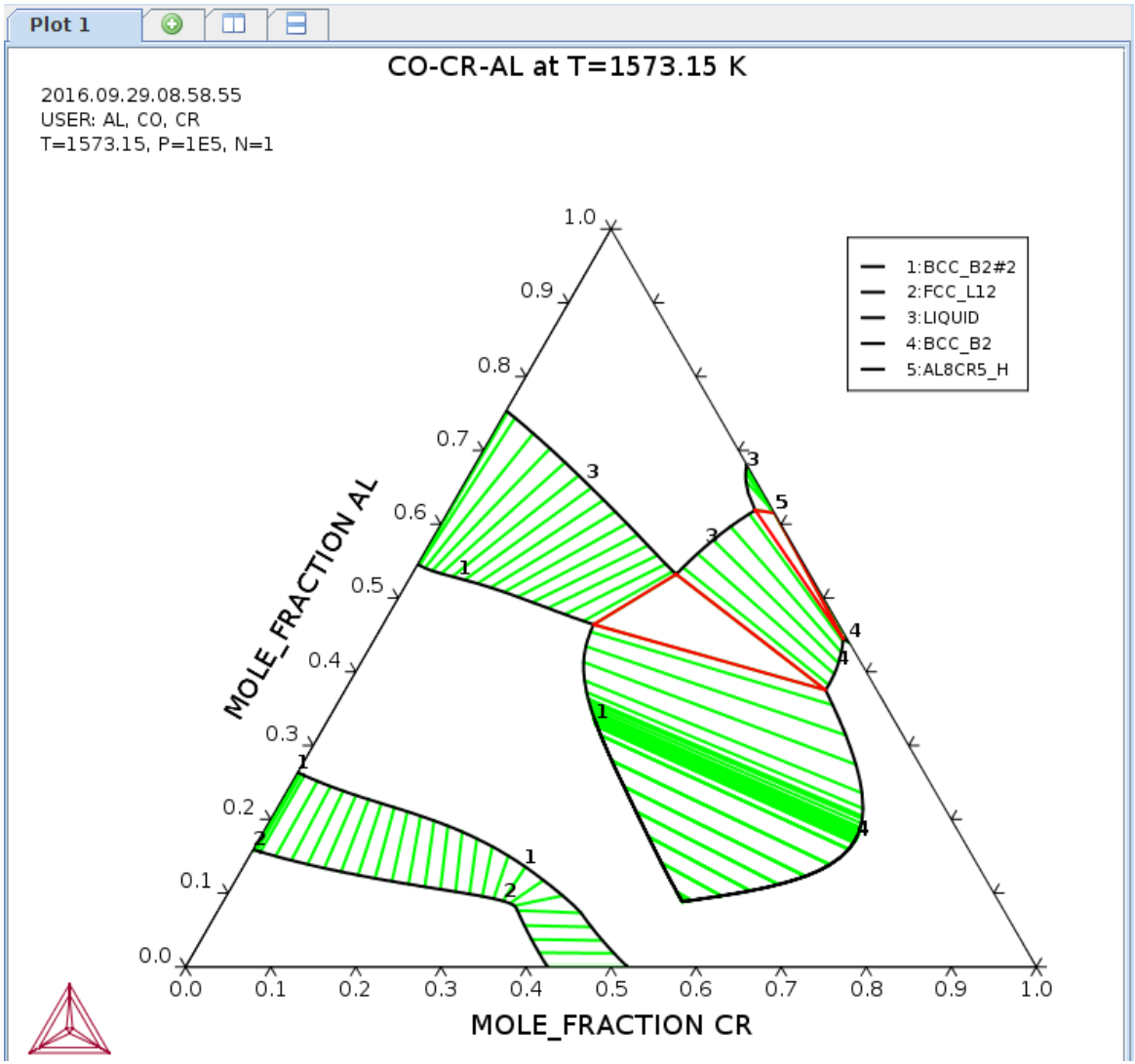
BCC_B2 décrit

- B2, le composé AlNi.
- A2, la solution solide base (Cr)

Transition de 2nd ordre

```
go ter
TCNI
Co Cr Al

1300
```



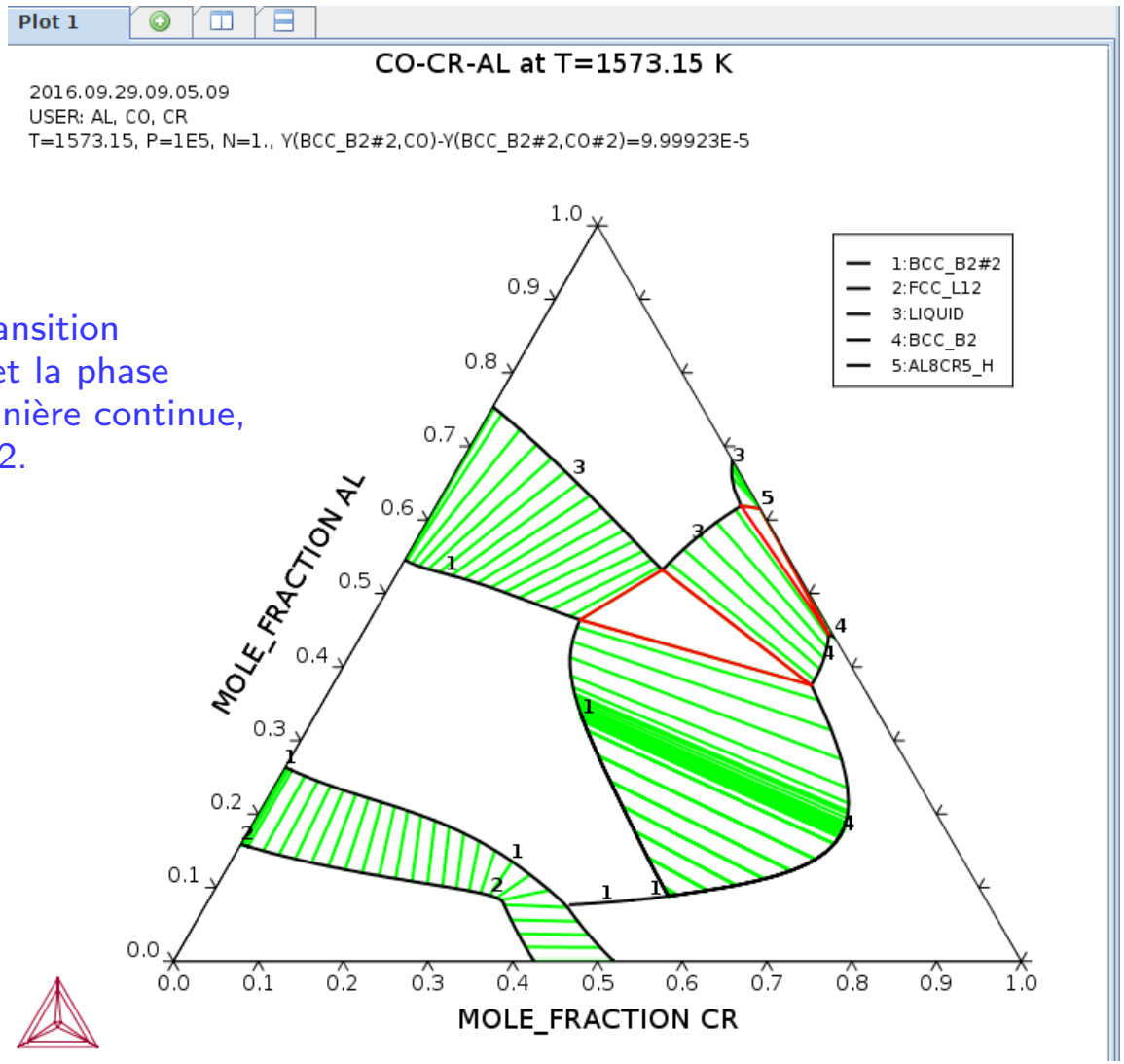
Transition de 2nd ordre

```
go ter
TCNI
Co Cr Al

1300

...
```

Il existe un domaine où la transition entre la phase ordonnée B2 et la phase désordonnée A2 a lieu de manière continue, sans domaine biphasé A2+B2.



Transition de 2nd ordre

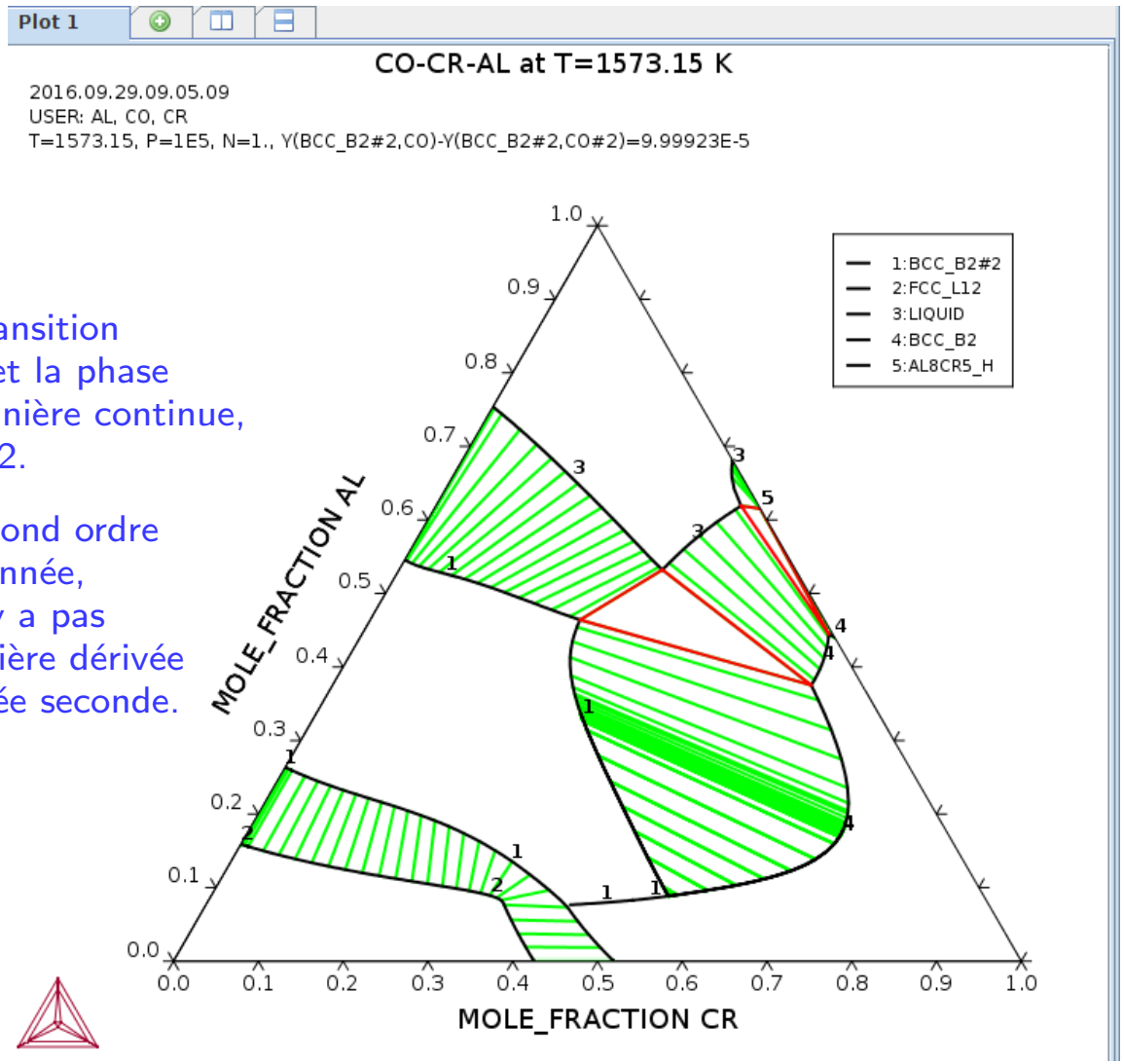
```
go ter
TCNI
Co Cr Al

1300

...
```

Il existe un domaine où la transition entre la phase ordonnée B2 et la phase désordonnée A2 a lieu de manière continue, sans domaine biphasé A2+B2.

On parle de transition de second ordre car pour une composition donnée, lors d'un échauffement, il n'y a pas d'effet notable pour H, première dérivée de G, mais pour le Cp, dérivée seconde.



Transition de 2nd ordre

```
go ter
TCNI
Co Cr Al

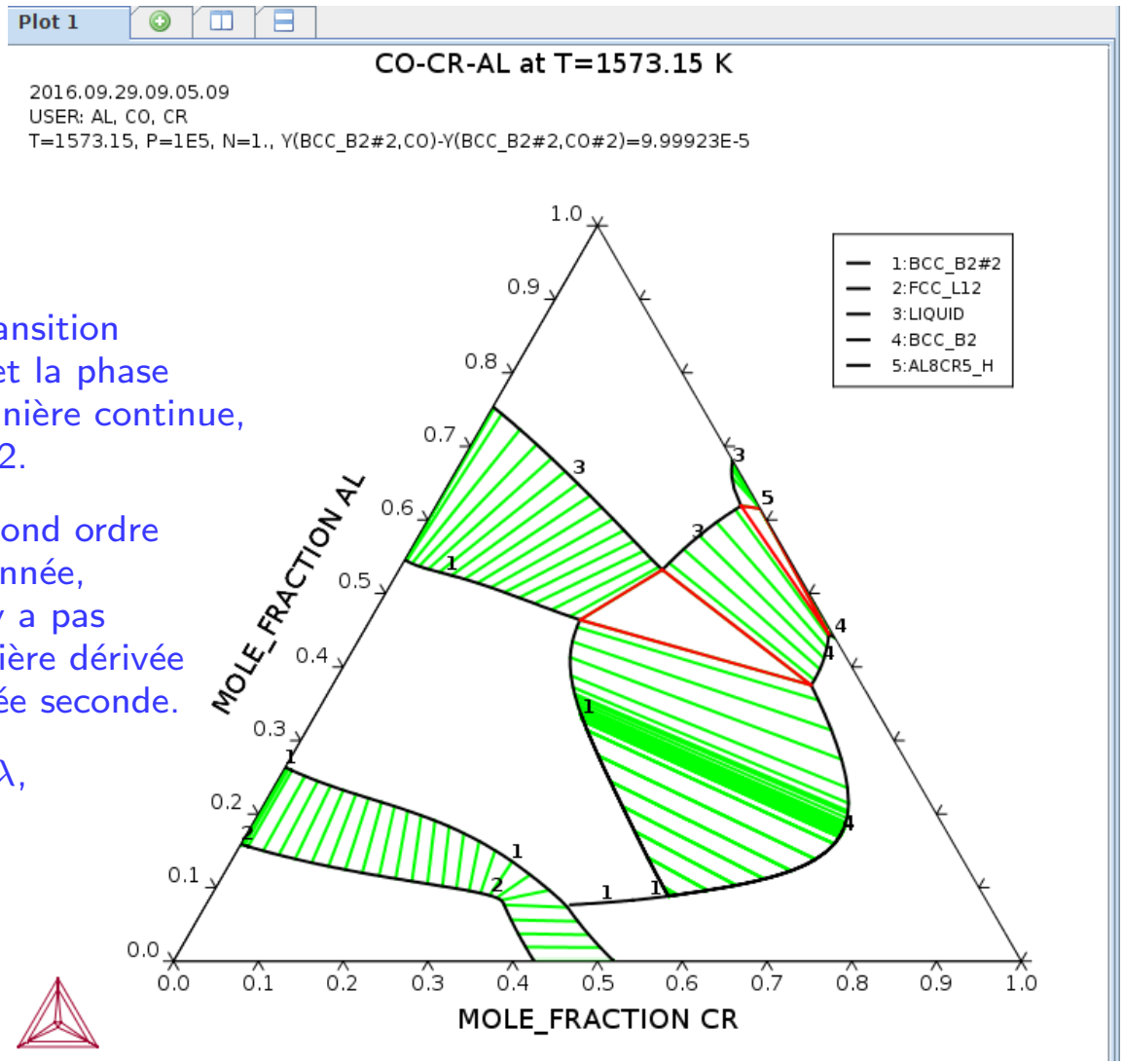
1300

...
```

Il existe un domaine où la transition entre la phase ordonnée B2 et la phase désordonnée A2 a lieu de manière continue, sans domaine biphasé A2+B2.

On parle de transition de second ordre car pour une composition donnée, lors d'un échauffement, il n'y a pas d'effet notable pour H, première dérivée de G, mais pour le Cp, dérivée seconde.

On parle aussi de transition λ, du fait de la forme du Cp lors d'une telle transition.

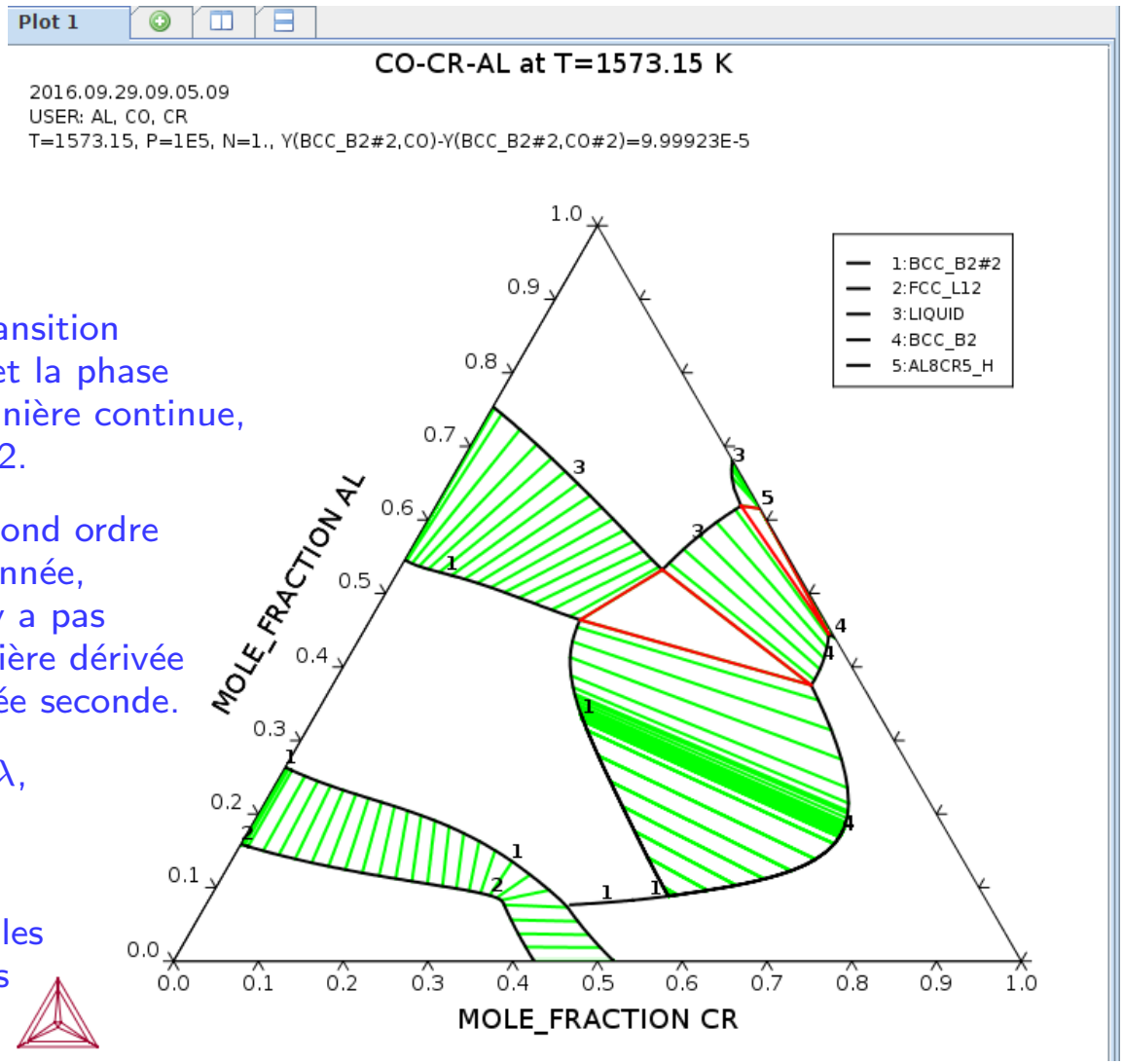


Transition de 2nd ordre

```
go ter
TCNI
Co Cr Al

1300

...
```



Il existe un domaine où la transition entre la phase ordonnée B2 et la phase désordonnée A2 a lieu de manière continue, sans domaine biphasé A2+B2.

On parle de transition de second ordre car pour une composition donnée, lors d'un échauffement, il n'y a pas d'effet notable pour H, première dérivée de G, mais pour le Cp, dérivée seconde.

On parle aussi de transition λ, du fait de la forme du Cp lors d'une telle transition.

La manière de calculer de telles transitions est présentée dans le cas du binaire Fe-Al par l'exemple `tcex16`.

Conclusion

- La base de données thermodynamiques commerciale TCNI permet de calculer des équilibres multicomposés d'intérêt dans le domaine des superalliages base Ni.
- Elle se singularise par
  - une description complète de l'ensemble des systèmes binaires constitutifs, permettant des calculs réalistes pour des compositions simplifiées ou très éloignées des compositions industrielles,
  - une description thermodynamique prenant en compte les relations crystallographiques d'ordre entre les phases A1/$L1_2$ et A2/B2, et en particulier les transitions de second ordre pour ces dernières.