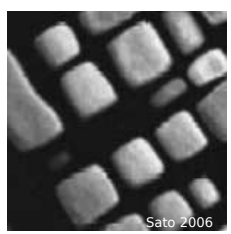
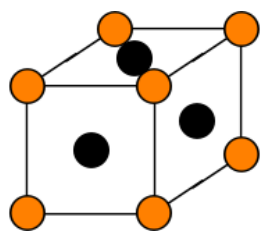
Mise en ordre

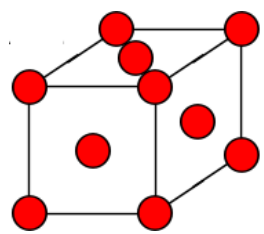
Nathalie Dupin

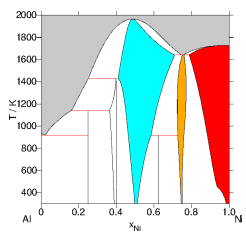
Calcul Thermodynamique

CIRIMAT, Toulouse, 28 mai 2015









Plan

- TCNI
  - généralités
  - fcc
  - MC
  - bcc
  - 2nd ordre
- 4 sous-réseaux
  - généralités
  - bcc
  - fcc
  - exercices

TCNI

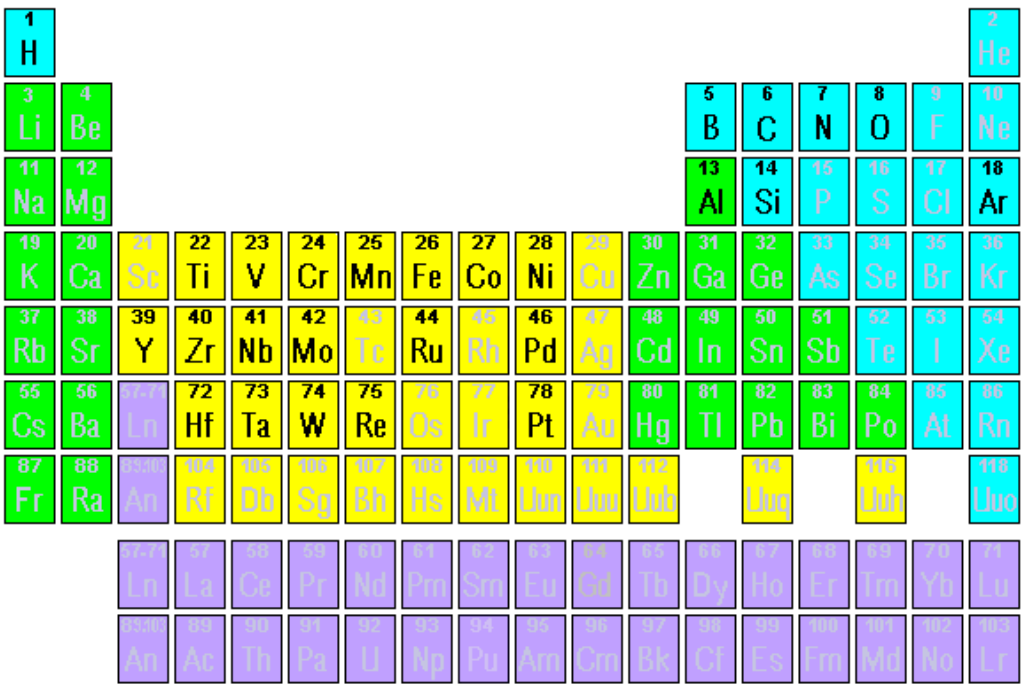
- Base de données commerciale développée par TCSAB dans le cadre d'une collaboration avec des partenaires industriels pour décrire les équilibres de phases dans les superalliages.

TCNI

- Base de données 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

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TCNI

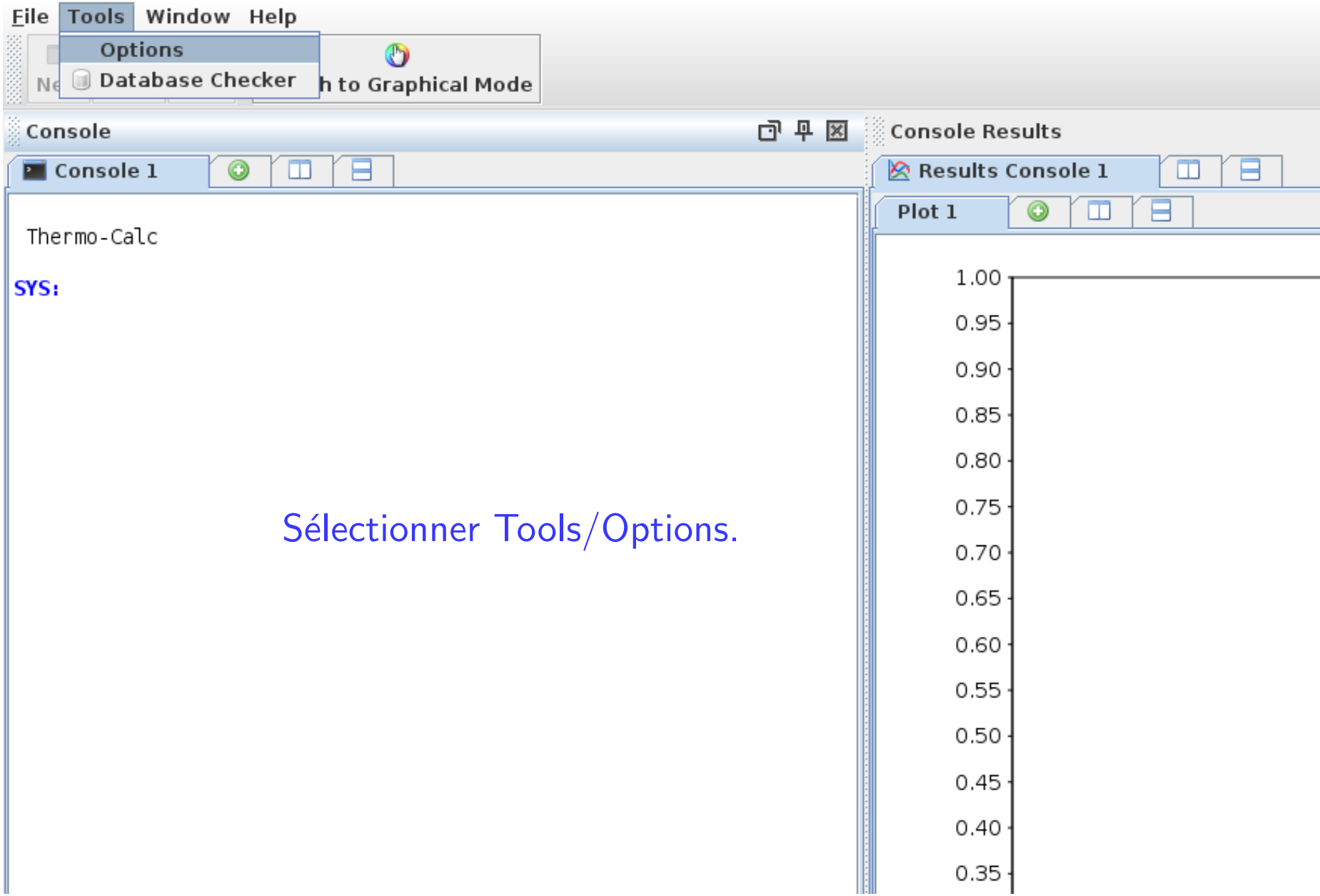
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- Seules les phases d'intérêt pour les alliages industriels sont extraites par défaut.

TCNI

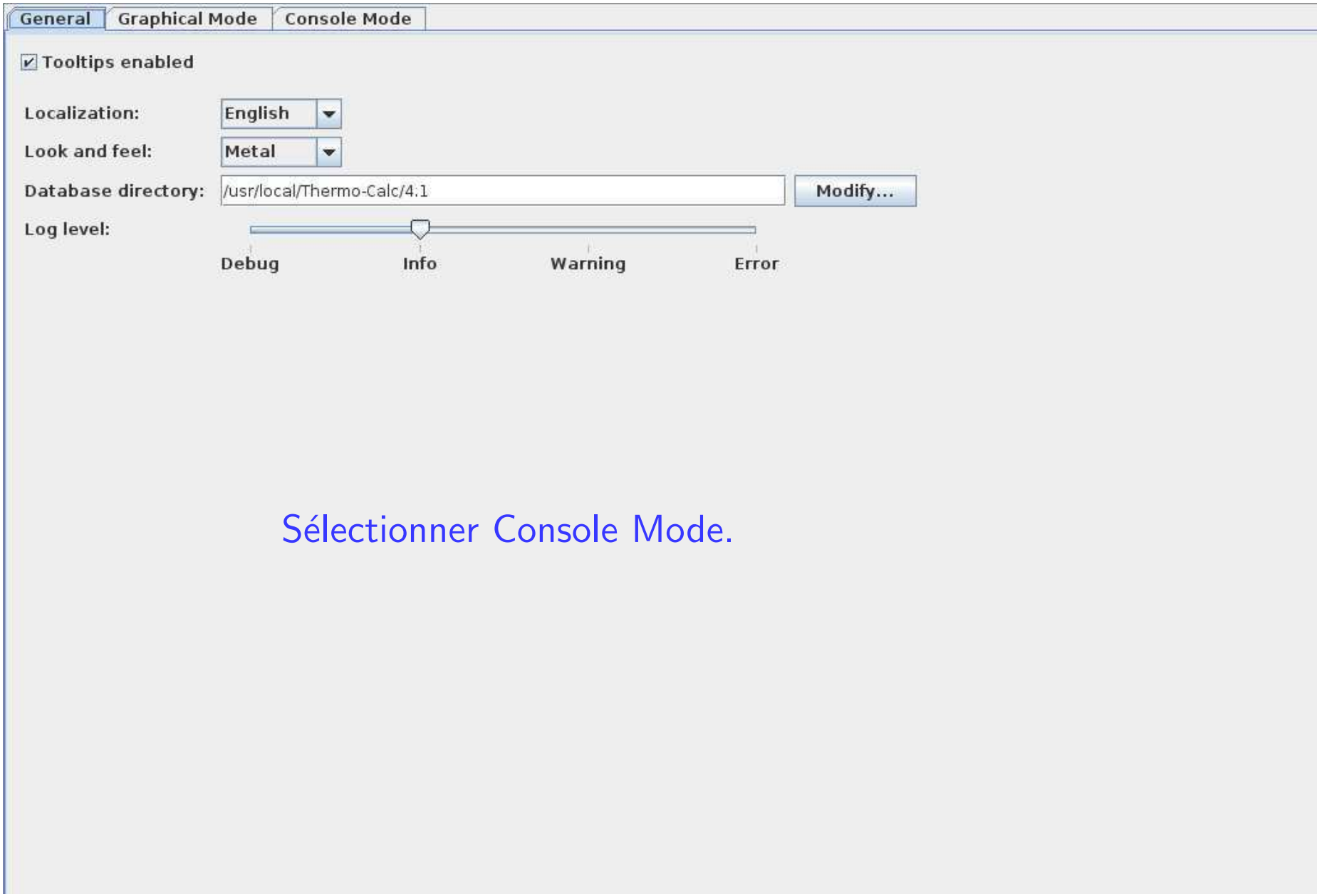
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- Seules les phases d'intérêt pour les alliages industriels sont extraites par défaut.
- Les descriptions complètes des systèmes binaires et des systèmes ternaires évalués sont accessibles en utilisant les modules `BINARY` et `TERNARY`.

TCNI

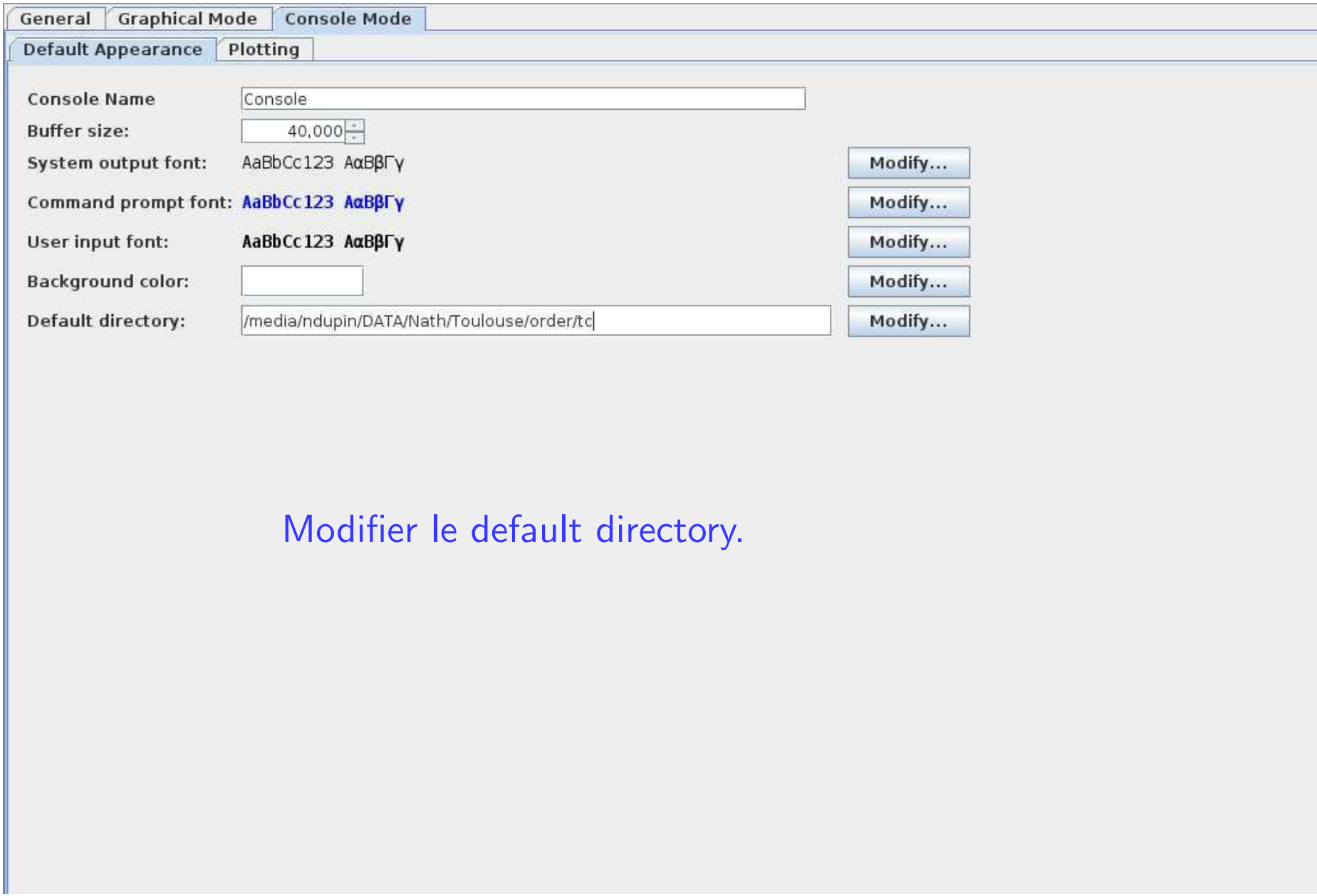
- Base de données commerciale développée par TCSAB dans le cadre d'une collaboration avec des partenaires industriels pour décrire les équilibres de phases dans les superalliages.
- Tous les binaires du système complexe Al-B-C-Co-Cr-Fe-Hf-Mn-Mo-N-Nb-Ni-O-Pd-Pt-Re-Ru-Si-Ta-Ti-V-W-Y-Zr sont décrits.
- 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 présentant des relations d'ordre $A1/L1_2$ et $A2/B2$.



Sélectionner Tools/Options.

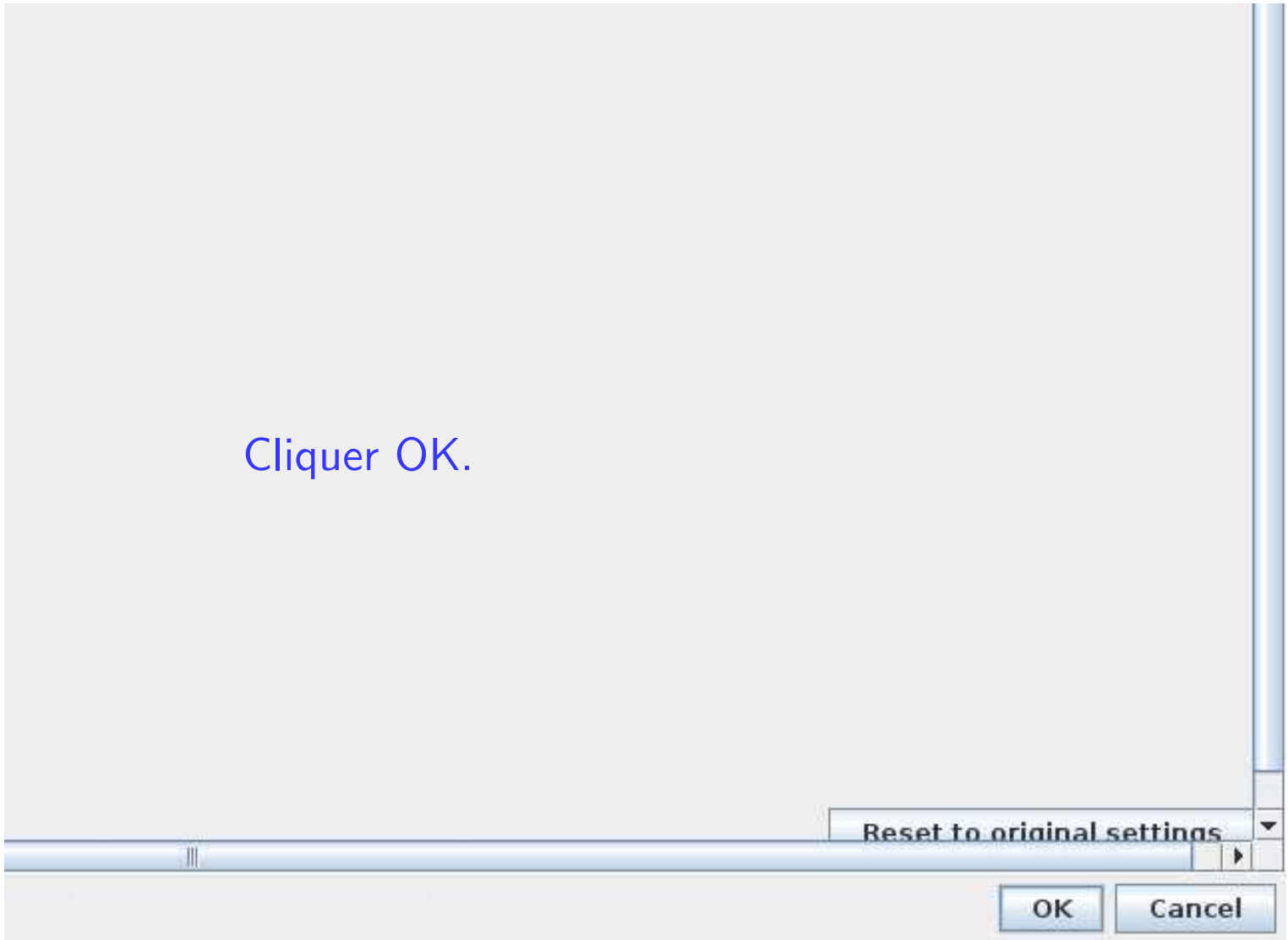


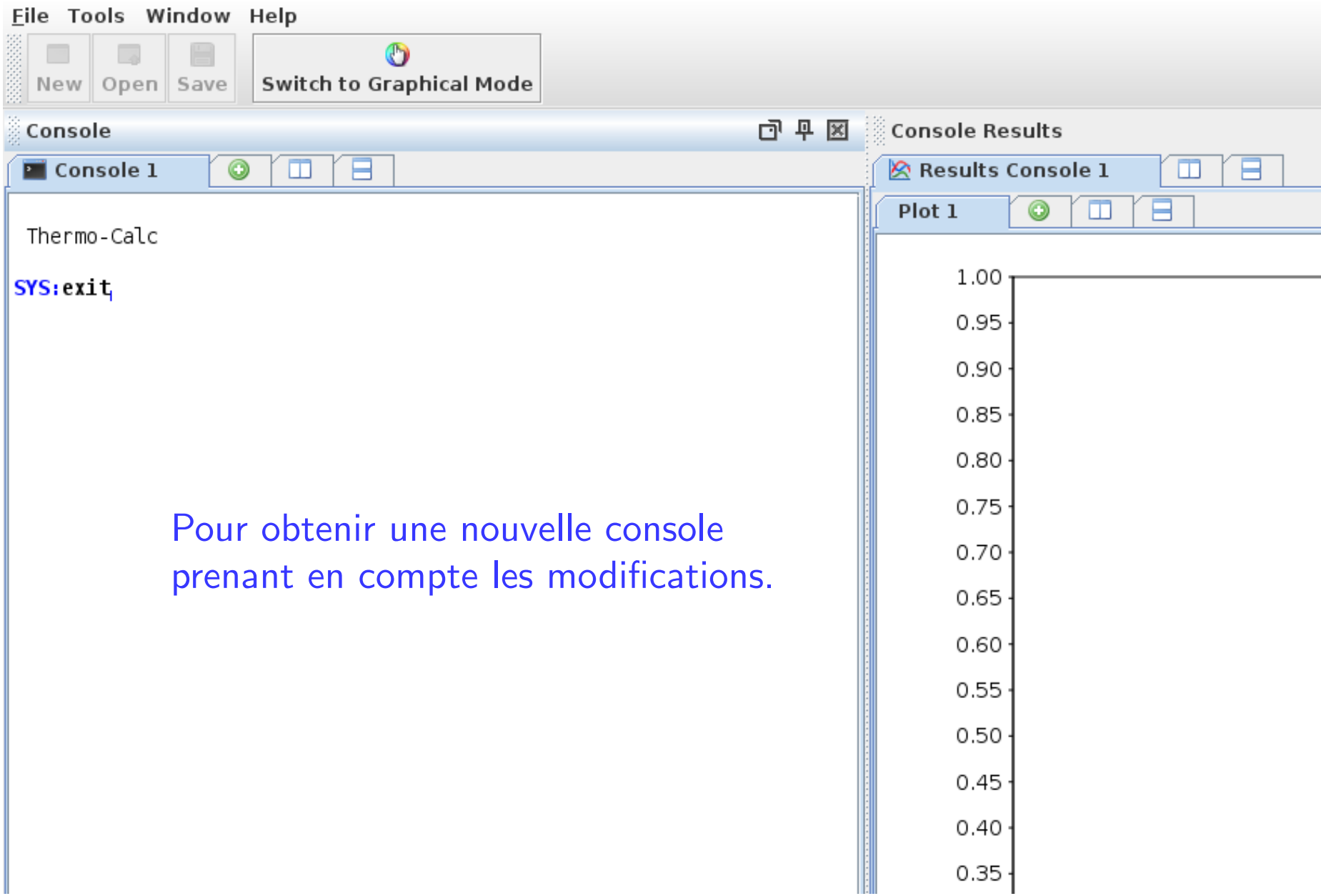
Sélectionner Console Mode.



Modifier le default directory.

Cliquer OK.



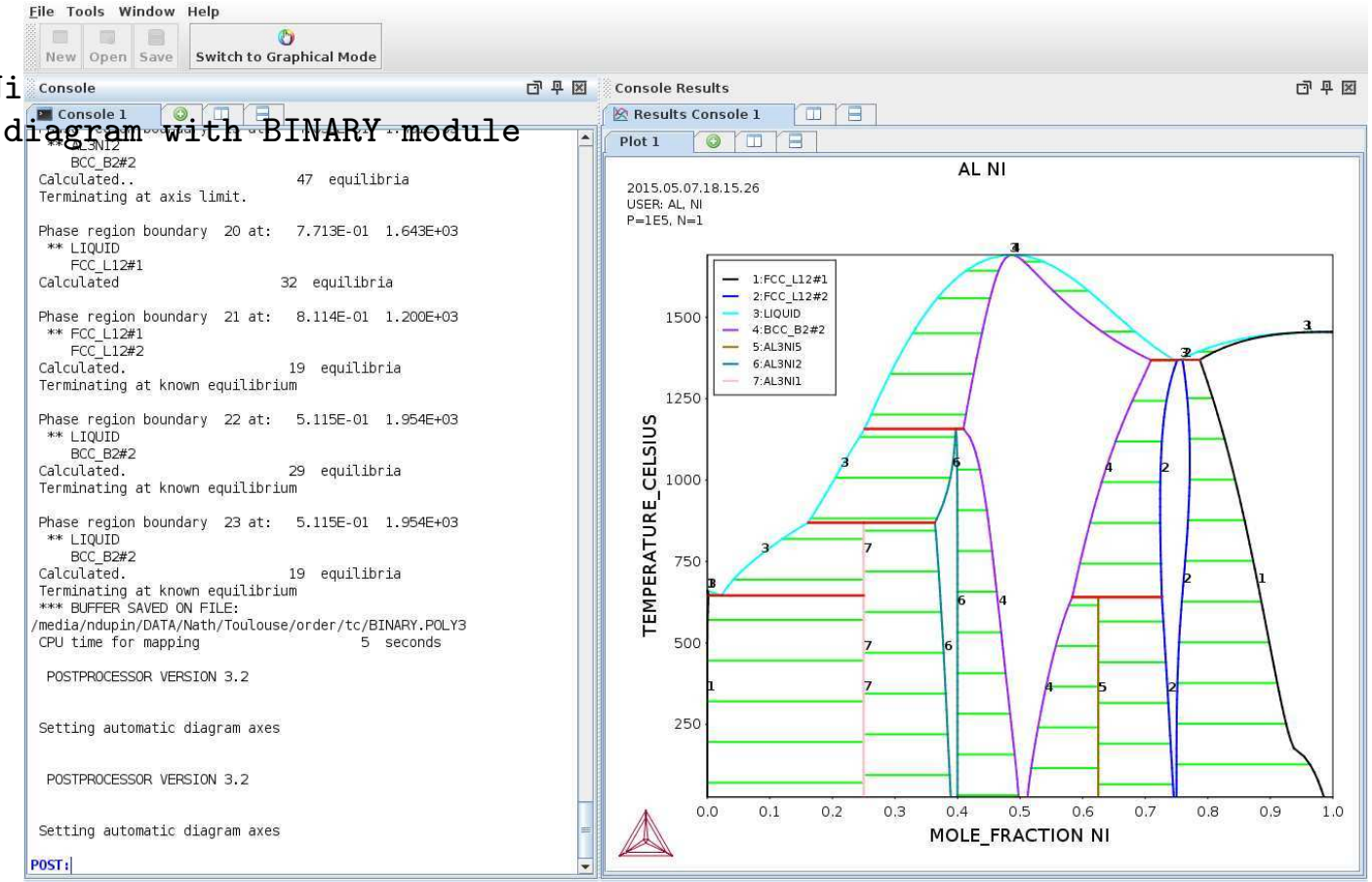

File Tools Window Help
New
Open
Save
Switch to Graphical Mode
Console
Console 1
Thermo-Calc
SYS:exit
Pour obtenir une nouvelle console
prenant en compte les modifications.
Console Results
Results Console 1
Plot 1
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35

Al-Ni

```
set_log Al-Ni
Al-Ni Phase diagram with BINARY module
go bin
TCNI
Al
Ni
```

Al-Ni

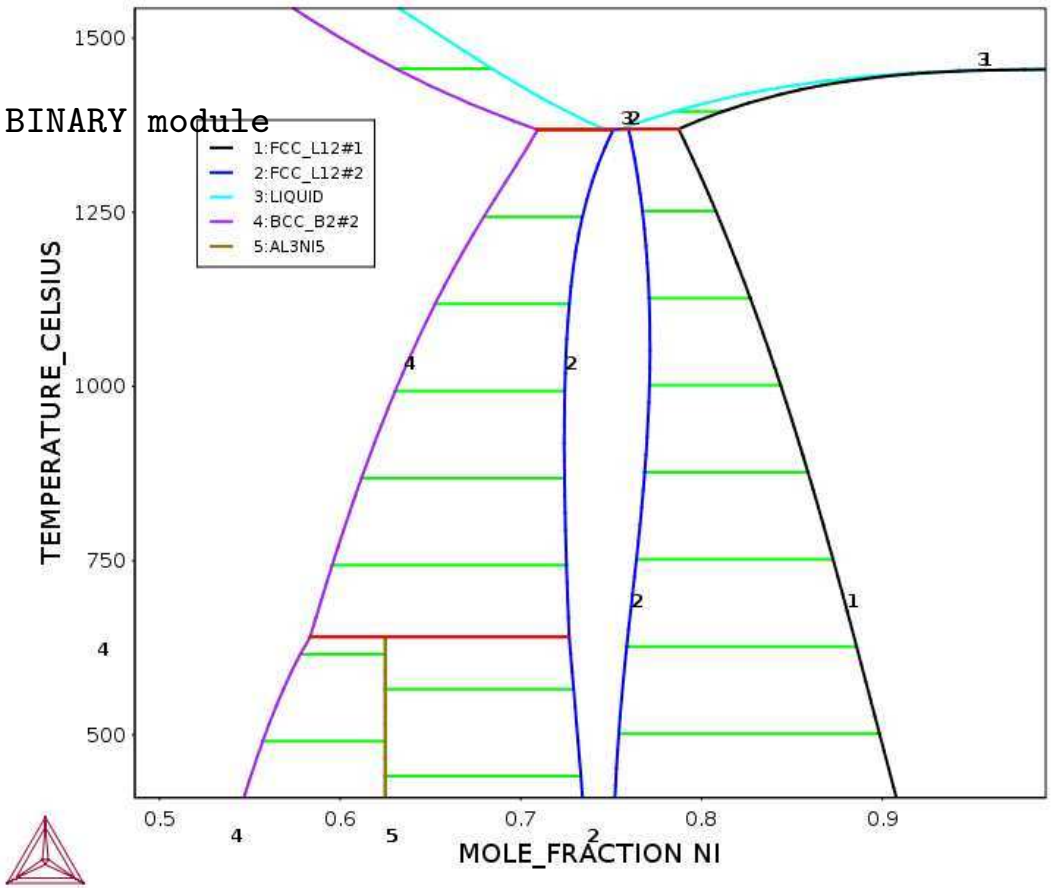
```
set_log Al-Ni
Al-Ni Phase diagram with BINARY module
go bin
TCNI
Al
Ni
```



Al-Ni

```
set_log Al-Ni
Al-Ni Phase diagram with BINARY module
go bin
TCNI
Al
Ni

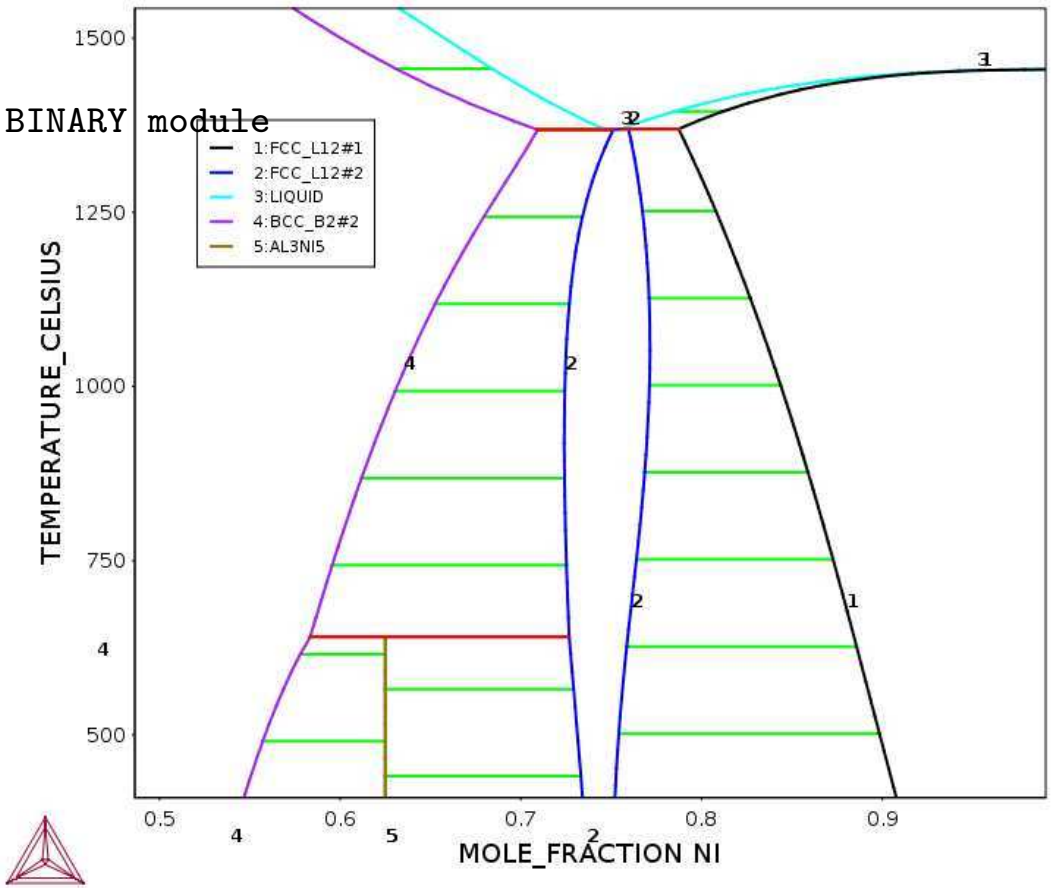
b
go poly
l_c
rea,,
s_c x(ni)=.8 t=1200
c_e
l_e
```



Al-Ni

```
set_log Al-Ni
Al-Ni Phase diagram with BINARY module
go bin
TCNI
Al
Ni

b
go poly
l_c
rea,,
s_c x(ni)=.8 t=1200
c_e
l_e
```



Al-Ni

```
set_log Al-Ni
Al-Ni Phase diagram with BINARY module
go bin
TCNI
Al
Ni

b
go poly
l_c
rea,,
s_c x(ni)=.8 t=1200
c_e
l_e
```

```
POST:b
 Current database: SGTE Unary (Pure Elements) TDB v5.1

 VA                       /-  DEFINED
SYS:go pol
POLY_3:l_c
 X(NI)=0.8, P=1E5, N=1, T=1200
 FIXED PHASES
 LIQUID=.2018557
 DEGREES OF FREEDOM -1
POLY_3:rea,,
POLY_3:s_c x(ni)=.8 t=1200
POLY_3:c_e
 Using global minimization procedure
Calculated         17829 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
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#1
 NI                     8.0000E-01  8.9691E-01 6.8371E-01 -3.7936E+03 FCC_A1#1

 FCC_L12#2                   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#1                   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
POLY_3:
```

Al-Ni

```
l_e

N
```

Al-Ni

```
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#1
 NI                     8.0000E-01  8.9691E-01 6.8371E-01 -3.7936E+03 FCC_A1#1

 FCC_L12#2                  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#1                  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
POLY_3:
```

Al-Ni

```
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

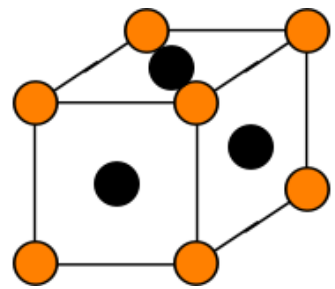
 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      2.0000E-01  1.0309E-01 1.7170E-06 -1.3245E+05 FCC_A1#1
 NI                      8.0000E-01  8.9691E-01 6.8371E-01 -3.7936E+03 FCC_A1#1

 FCC_L12#2                   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#1                   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
POLY_3:
```

l_e

N



Al-Ni

```
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

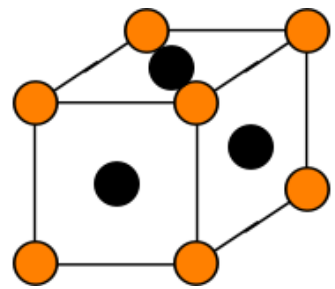
 Conditions:
 X(NI)=0.8, P=1E5, N=1, T=1200
 DEGREES OF FREEDOM 0

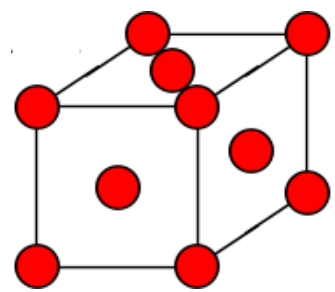
 Temperature   1200.00 K (   926.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.23484E+01
 Total Gibbs energy -8.75017E+04,  Enthalpy -5.40654E+03,  Volume  7.08284E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      2.0000E-01  1.0309E-01 1.7170E-06 -1.3245E+05 FCC_A1#1
 NI                      8.0000E-01  8.9691E-01 6.8371E-01 -3.7936E+03 FCC_A1#1

 FCC_L12#2                   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#1                   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
POLY_3:
```





Al-Ni

```
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

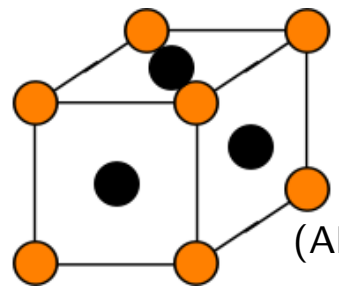
 Conditions:
 X(NI)=0.8, P=1E5, N=1, T=1200
 DEGREES OF FREEDOM 0

 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

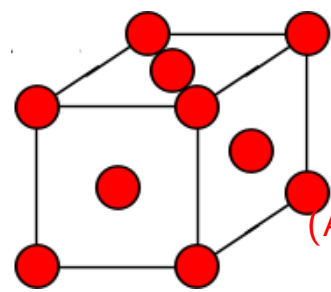
 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      2.0000E-01  1.0309E-01 1.7170E-06 -1.3245E+05 FCC_A1#1
 NI                      8.0000E-01  8.9691E-01 6.8371E-01 -3.7936E+03 FCC_A1#1

 FCC_L12#2                   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#1                   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
POLY_3:
```



$(Al_{0.005}Ni_{0.995})_{0.75}$ $(Al_{0.907}Ni_{0.093})_{0.25}$



$(Al_{0.147}Ni_{0.853})_{0.75}$ $(Al_{0.147}Ni_{0.853})_{0.25}$

Al-Ni

```
show y(fcc_l12,*) y(fcc_l12#2,*)
```

Al-Ni

```
show y(fcc_l12,*) y(fcc_l12#2,*)
```

```
POLY_3:show y(fcc_l12,*) y(fcc_l12#2,*)
 Y(FCC_L12#1,AL)=0.14701799, Y(FCC_L12#1,NI)=0.85298201,
    Y(FCC_L12#1,AL#2)=0.14701799, Y(FCC_L12#1,NI#2)=0.85298201,
    Y(FCC_L12#1,VA#3)=1
 Y(FCC_L12#2,AL)=4.6250162E-3, Y(FCC_L12#2,NI)=0.99537498,
    Y(FCC_L12#2,AL#2)=0.90672575, Y(FCC_L12#2,NI#2)=9.3274247E-2,
    Y(FCC_L12#2,VA#3)=1
POLY_3:
```

Al-Ni

```
show y(fcc_l12,*) y(fcc_l12#2,*)

show y(fcc_l12,ni) y(fcc_l12,ni#2) y(FCC_L12#2,ni) y(FCC_L12#2,ni#2)
```

Al-Ni

```
show y(fcc_l12,*) y(fcc_l12#2,*)

show y(fcc_l12,ni) y(fcc_l12,ni#2) y(FCC_L12#2,ni) y(FCC_L12#2,ni#2)
```

```
POLY_3:show y(fcc_l12,ni) y(fcc_l12,ni#2) y(FCC_L12#2,ni) y(FCC_L12#2,ni#2)
 Y(FCC_L12#1,NI)=0.85298201
 Y(FCC_L12#1,NI#2)=0.85298201
 Y(FCC_L12#2,NI)=0.99537498
 Y(FCC_L12#2,NI#2)=9.3274247E-2
POLY_3:
```

Al-Ni

```
show y(fcc_l12,*) y(fcc_l12#2,*)

show y(fcc_l12,ni) y(fcc_l12,ni#2) y(FCC_L12#2,ni) y(FCC_L12#2,ni#2)
```

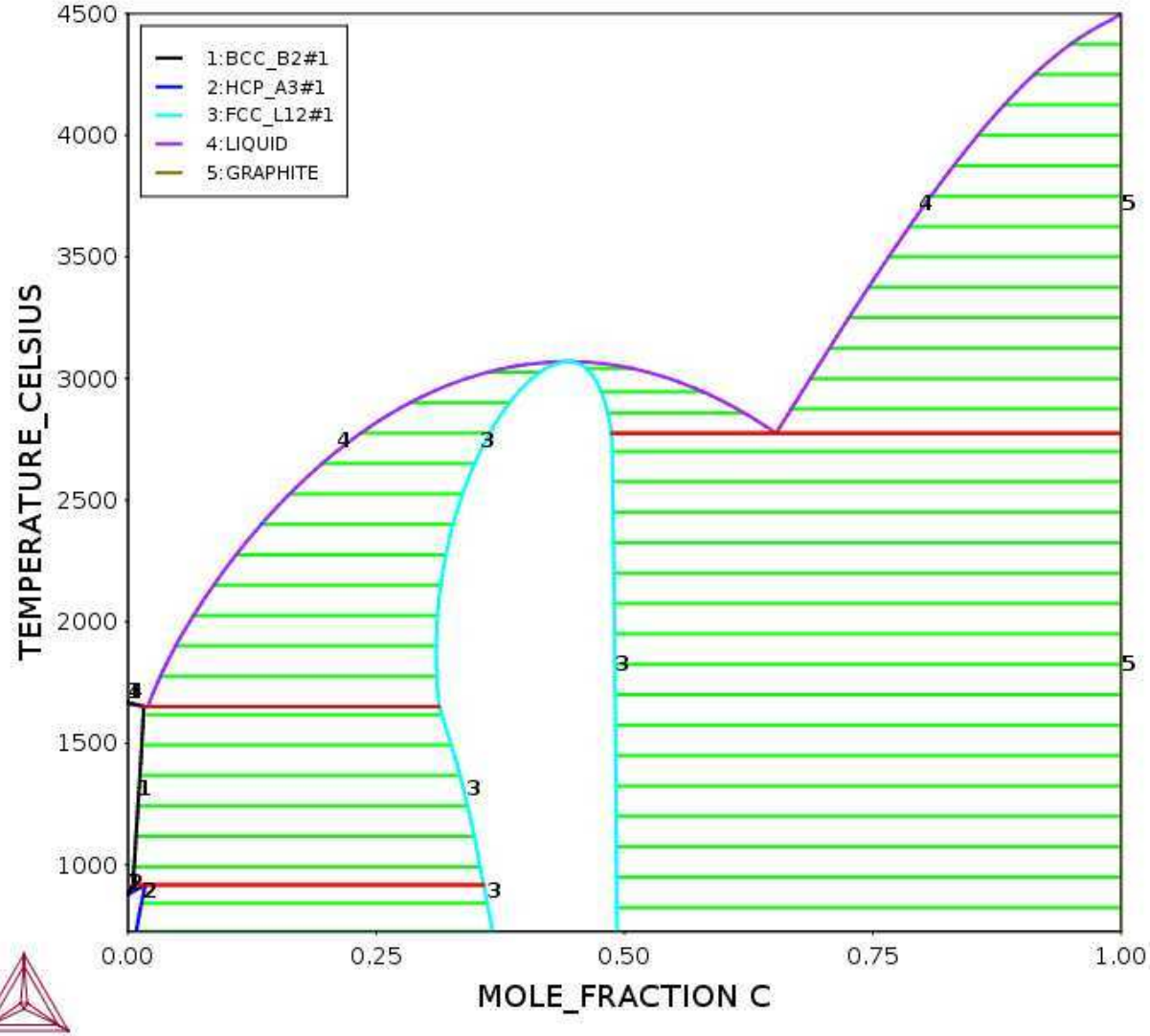
- Les phases γ, A1, et γ', $L1_2$, sont décrites avec une seule équation, fonction de l'occupation des sous-réseaux.
- Les différentes constitutions sont identifiées par des suffixes `#n`.
- En général `FCC_L12#1` est désordonnée et `FCC_L12#2` ordonnée.
- Ce n'est toutefois pas toujours le cas, en particulier quand la `global minimisation` est activée.
- La seule manière d'identitifier une phase est de vérifier l'occupation de ses sous-réseaux.

Ti-C

```
go bin
TCNI
Ti C
```

Ti-C

```
go bin
TCNI
Ti C
```

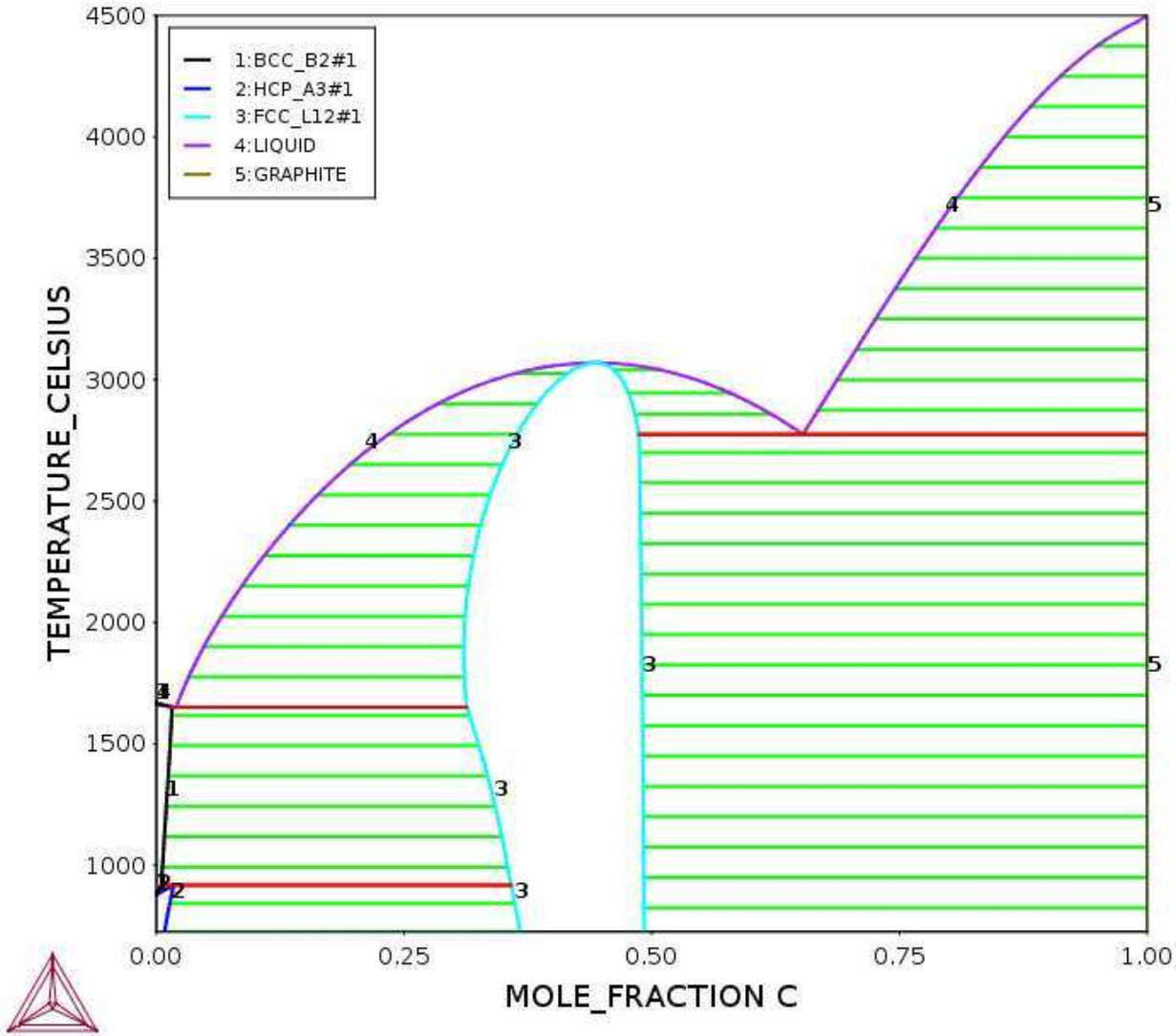


Ti-C

```
go bin
TCNI
Ti C


b
go pol
l_c
rea,,
s_c x(ti)=.6
c_e
l_e

N
```



Ti-C

```
go bin
TCNI
Ti C


b
go pol
l_c
rea,,
s_c x(ti)=.6
c_e
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(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.sta
 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#1                    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
POLY_3:
```

Ti-C

```
go bin
TCNI
Ti C


b
go pol
l_c
rea,,
s_c x(ti)=.6
c_e
l_e

N
```

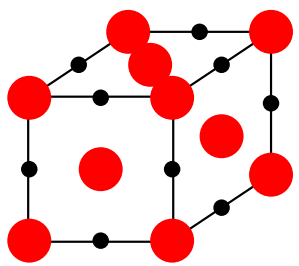
```
POLY_3:l_e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:n
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 X(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.sta
 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#1                    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
POLY_3:
```



B1 (Ti)($C_{0.666}\square_{0.333}$)

Ti-C

```
go bin
TCNI
Ti C


b
go pol
l_c
rea,,
s_c x(ti)=.6
c_e
l_e

N
```

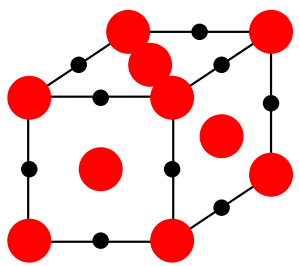
```
POLY_3:l_e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:n
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 X(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.sta
 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#1                    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
POLY_3:
```



B1 (Ti)($C_{0.666}\square_{0.333}$)

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, N=1, X(AL)=5E-2, X(TI)=0.1, X(C)=1E-2, 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  5.55568E+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                   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                   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#1                   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.
- Sa composition renseigne sur sa nature. Seule sa constitution permet de discriminer sans ambigüité γ et γ'.

```
Conditions:
P=1E5, N=1, X(AL)=5E-2, X(TI)=0.1, X(C)=1E-2, 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  5.55568E+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                   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                   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

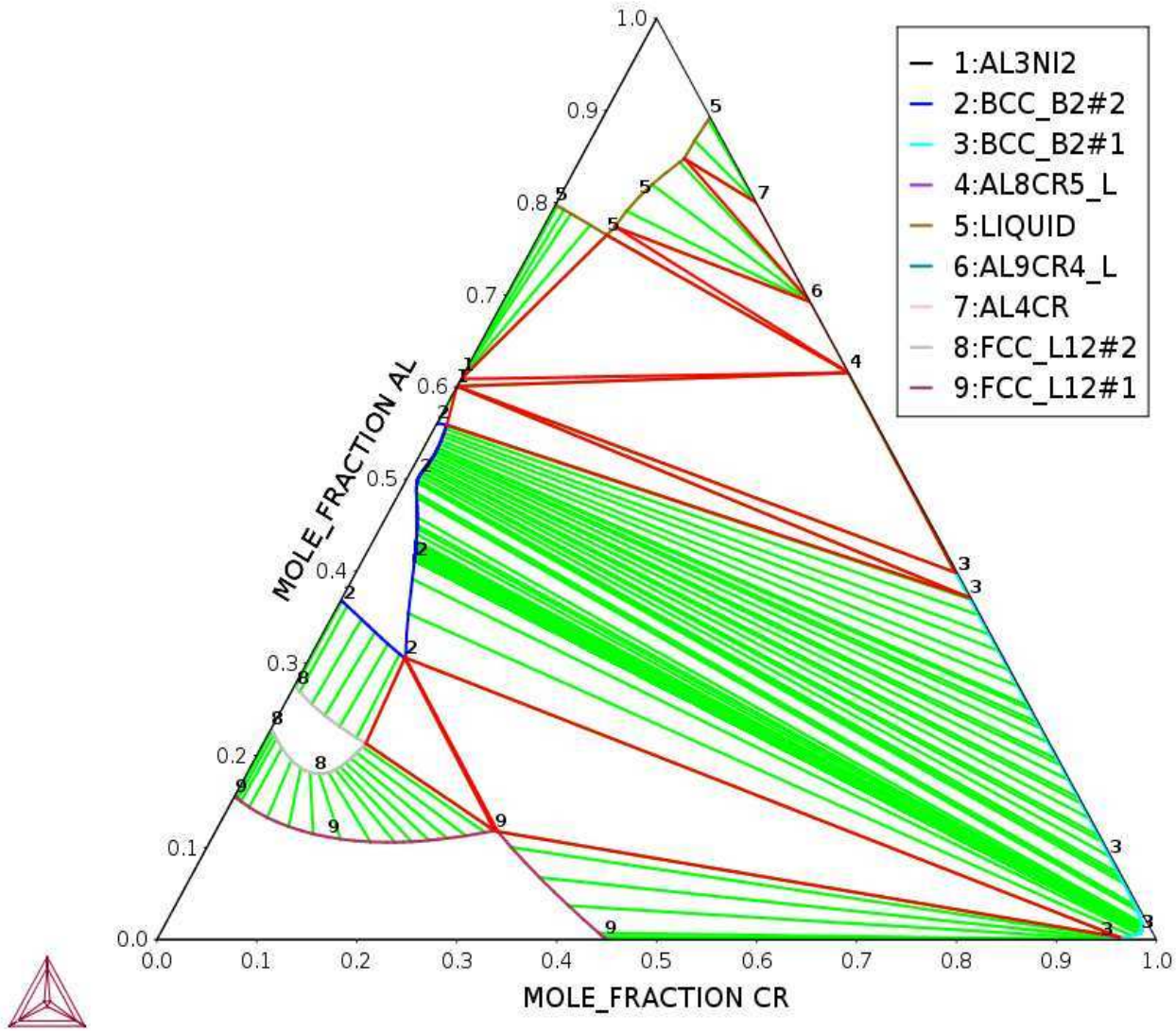
FCC_L12#1                   Status ENTERED     Driving force  0.0000E+00
Moles 1.6578E-02, Mass 5.0634E-01, Volume fraction 1.5036E-02  Mass fractions:
TI  8.09804E-01  C   1.90079E-01  NI  1.16846E-04  AL  1.16538E-11
Constitution:
Sublattice  1,  Number of sites  7.5000E-01
TI  9.99882E-01  NI  1.17698E-04  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-Cr-Ni

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

Al-Cr-Ni

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



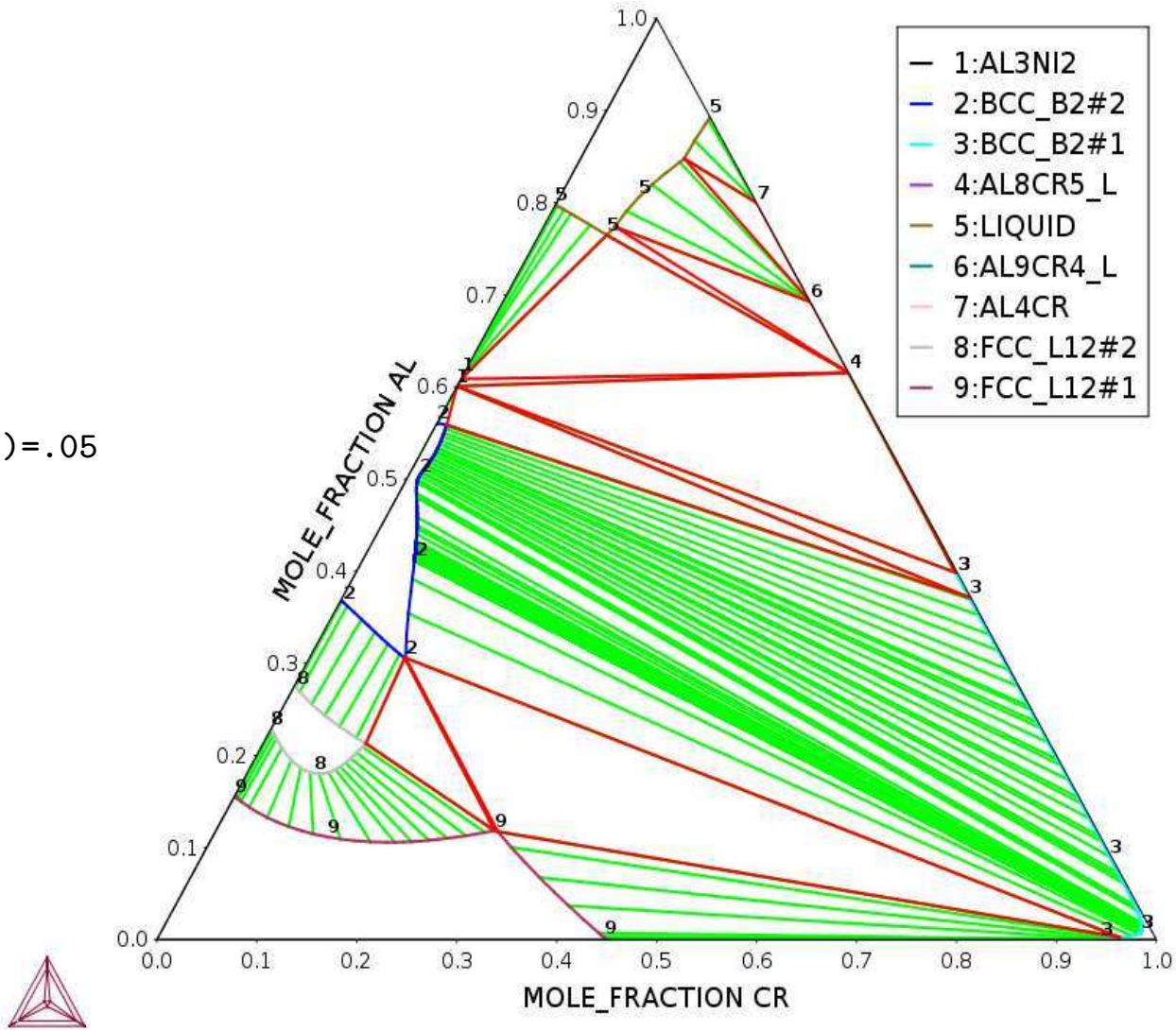
Al-Cr-Ni

```
go ter
TCNI
Ni Cr Al



b
go pol
l_c
rea,,
s_c x(cr)=.9 x(ni)=.05
c_e
l_e

N
```



Al-Cr-Ni

```
go ter
TCNI
Ni Cr Al



b
go pol
l_c
rea,,
s_c x(cr)=.9 x(ni)=.05
c_e
l_e

N
```

```
POLY_3:s_c x(cr)=.9 x(ni)=.05
POLY_3:c_e
 Using global minimization procedure
Calculated         22136 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:l_e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWNS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 T=1273.15, P=1E5, N=1, X(CR)=0.9, X(NI)=5E-2
 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  5.10800E+01
 Total Gibbs energy -5.98451E+04,  Enthalpy  2.35899E+04,  Volume  7.46897E-06

 Component              Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                     5.0000E-02  2.6412E-02 1.3382E-06 -1.4316E+05 SER
 CR                     9.0000E-01  9.1614E-01 6.4641E-03 -5.3367E+04 SER
 NI                     5.0000E-02  5.7449E-02 1.5109E-04 -9.3128E+04 SER

 BCC_B2#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 9.1612E-01, Mass 4.7361E+01, Volume fraction 9.1536E-01  Mass fractions:
 CR  9.84592E-01  NI  8.16449E-03  AL  7.24390E-03
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 CR  9.78929E-01  AL  1.38792E-02  NI  7.19167E-03  VA  1.07384E-09
 Sublattice  2,  Number of sites  5.0000E-01
 CR  9.78929E-01  AL  1.38792E-02  NI  7.19167E-03  VA  1.07384E-09
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00

 BCC_B2#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 8.3882E-02, Mass 3.7195E+00, Volume fraction 8.4643E-02  Mass fractions:
 NI  6.85000E-01  AL  2.70477E-01  CR  4.45237E-02
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 AL  8.88546E-01  CR  7.01005E-02  NI  4.13540E-02  VA  1.43302E-12
 Sublattice  2,  Number of sites  5.0000E-01
 NI  9.93215E-01  CR  5.80168E-03  VA  9.65453E-04  AL  1.79916E-05
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY_3:
```

Al-Cr-Ni

```
go ter
TCNI
Ni Cr Al



b
go pol
l_c
rea,,
s_c x(cr)=.9 x(ni)=.05
c_e
l_e

N
```

```
POLY_3:s_c x(cr)=.9 x(ni)=.05
POLY_3:c_e
 Using global minimization procedure
Calculated         22136 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:l_e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWNS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 T=1273.15, P=1E5, N=1, X(CR)=0.9, X(NI)=5E-2
 DEGREES OF FREEDOM 0

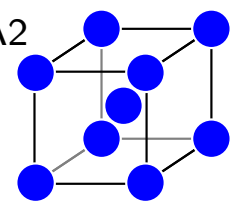
 Temperature   1273.15 K (  1000.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.10800E+01
 Total Gibbs energy -5.98451E+04,  Enthalpy  2.35899E+04,  Volume  7.46897E-06

 Component              Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                     5.0000E-02  2.6412E-02 1.3382E-06 -1.4316E+05 SER
 CR                     9.0000E-01  9.1614E-01 6.4641E-03 -5.3367E+04 SER
 NI                     5.0000E-02  5.7449E-02 1.5109E-04 -9.3128E+04 SER

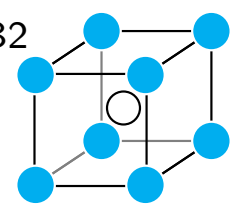
 BCC_B2#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 9.1612E-01, Mass 4.7361E+01, Volume fraction 9.1536E-01  Mass fractions:
 CR  9.84592E-01  NI  8.16449E-03  AL  7.24390E-03
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 CR  9.78929E-01  AL  1.38792E-02  NI  7.19167E-03  VA  1.07384E-09
 Sublattice  2,  Number of sites  5.0000E-01
 CR  9.78929E-01  AL  1.38792E-02  NI  7.19167E-03  VA  1.07384E-09
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00

 BCC_B2#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 8.3882E-02, Mass 3.7195E+00, Volume fraction 8.4643E-02  Mass fractions:
 NI  6.85000E-01  AL  2.70477E-01  CR  4.45237E-02
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 AL  8.88546E-01  CR  7.01005E-02  NI  4.13540E-02  VA  1.43302E-12
 Sublattice  2,  Number of sites  5.0000E-01
 NI  9.93215E-01  CR  5.80168E-03  VA  9.65453E-04  AL  1.79916E-05
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY_3:
```

A2



B2



Al-Cr-Ni

```
go ter
TCNI
Ni Cr Al



b
go pol
l_c
rea,,
s_c x(cr)=.9 x(ni)=.05
c_e
l_e

N
```

```
POLY_3:s_c x(cr)=.9 x(ni)=.05
POLY_3:c_e
 Using global minimization procedure
Calculated         22136 grid points in             0 s
Found the set of lowest grid points in              0 s
 Calculated POLY solution       0 s, total time     0  s
POLY_3:l_e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWNS/:
 Output from POLY-3, equilibrium =     1, label A0  , database: USER

 Conditions:
 T=1273.15, P=1E5, N=1, X(CR)=0.9, X(NI)=5E-2
 DEGREES OF FREEDOM 0

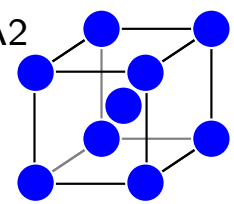
 Temperature   1273.15 K (  1000.00 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  5.10800E+01
 Total Gibbs energy -5.98451E+04,  Enthalpy  2.35899E+04,  Volume  7.46897E-06

 Component              Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                     5.0000E-02  2.6412E-02 1.3382E-06 -1.4316E+05 SER
 CR                     9.0000E-01  9.1614E-01 6.4641E-03 -5.3367E+04 SER
 NI                     5.0000E-02  5.7449E-02 1.5109E-04 -9.3128E+04 SER

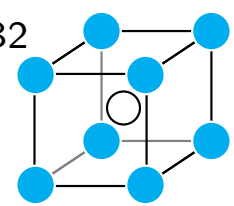
 BCC_B2#1                    Status ENTERED     Driving force  0.0000E+00
 Moles 9.1612E-01, Mass 4.7361E+01, Volume fraction 9.1536E-01  Mass fractions:
 CR  9.84592E-01  NI  8.16449E-03  AL  7.24390E-03
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 CR  9.78929E-01  AL  1.38792E-02  NI  7.19167E-03  VA  1.07384E-09
 Sublattice  2,  Number of sites  5.0000E-01
 CR  9.78929E-01  AL  1.38792E-02  NI  7.19167E-03  VA  1.07384E-09
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00

 BCC_B2#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 8.3882E-02, Mass 3.7195E+00, Volume fraction 8.4643E-02  Mass fractions:
 NI  6.85000E-01  AL  2.70477E-01  CR  4.45237E-02
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 AL  8.88546E-01  CR  7.01005E-02  NI  4.13540E-02  VA  1.43302E-12
 Sublattice  2,  Number of sites  5.0000E-01
 NI  9.93215E-01  CR  5.80168E-03  VA  9.65453E-04  AL  1.79916E-05
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY_3:
```

A2



B2



BCC_B2 décrit

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

Al-Co-Cr à 1300 °C

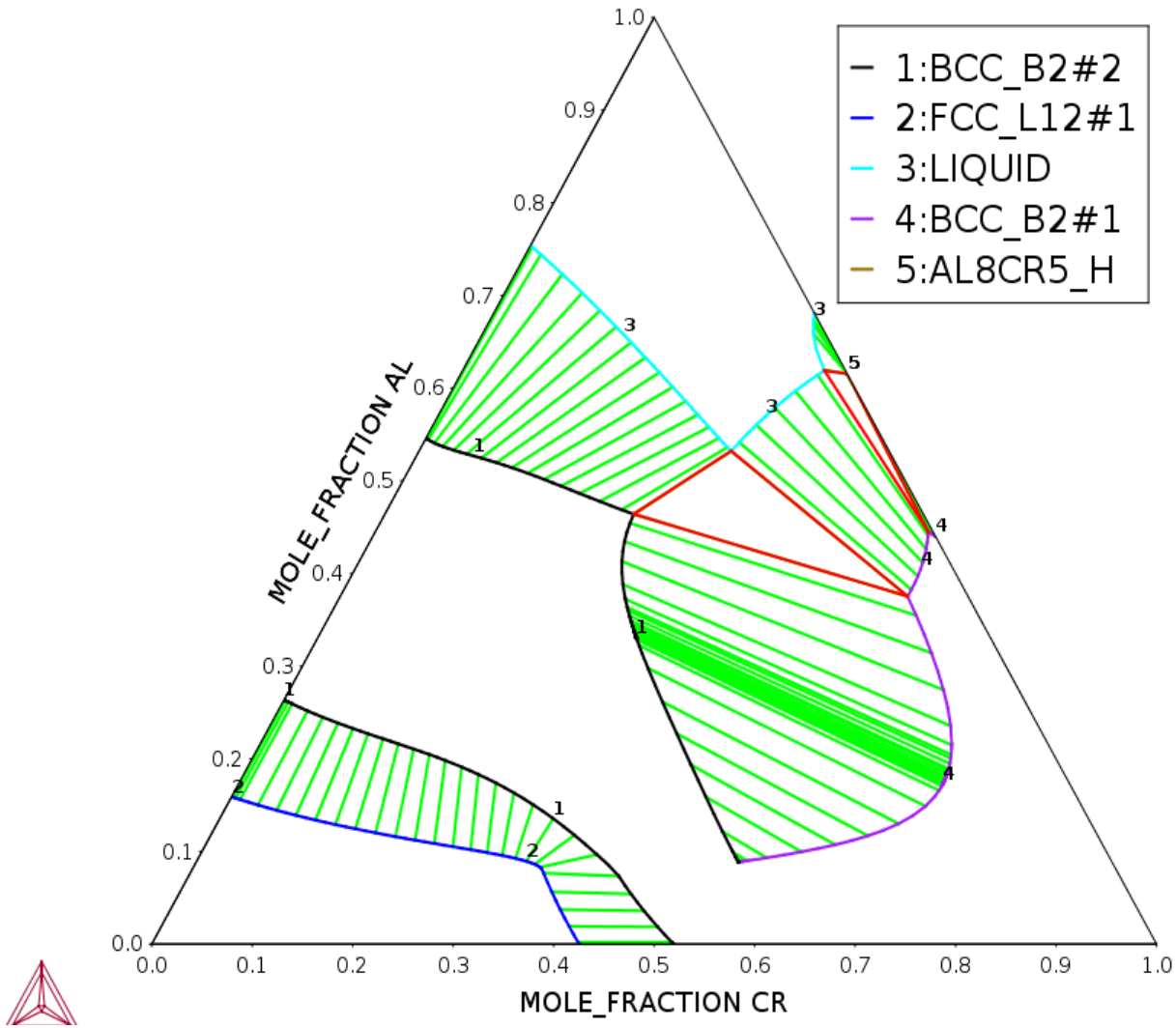
```
go ter
TCNI
Co Cr Al

1300
```

Al-Co-Cr à 1300 °C

```
go ter
TCNI
Co Cr Al

1300
```

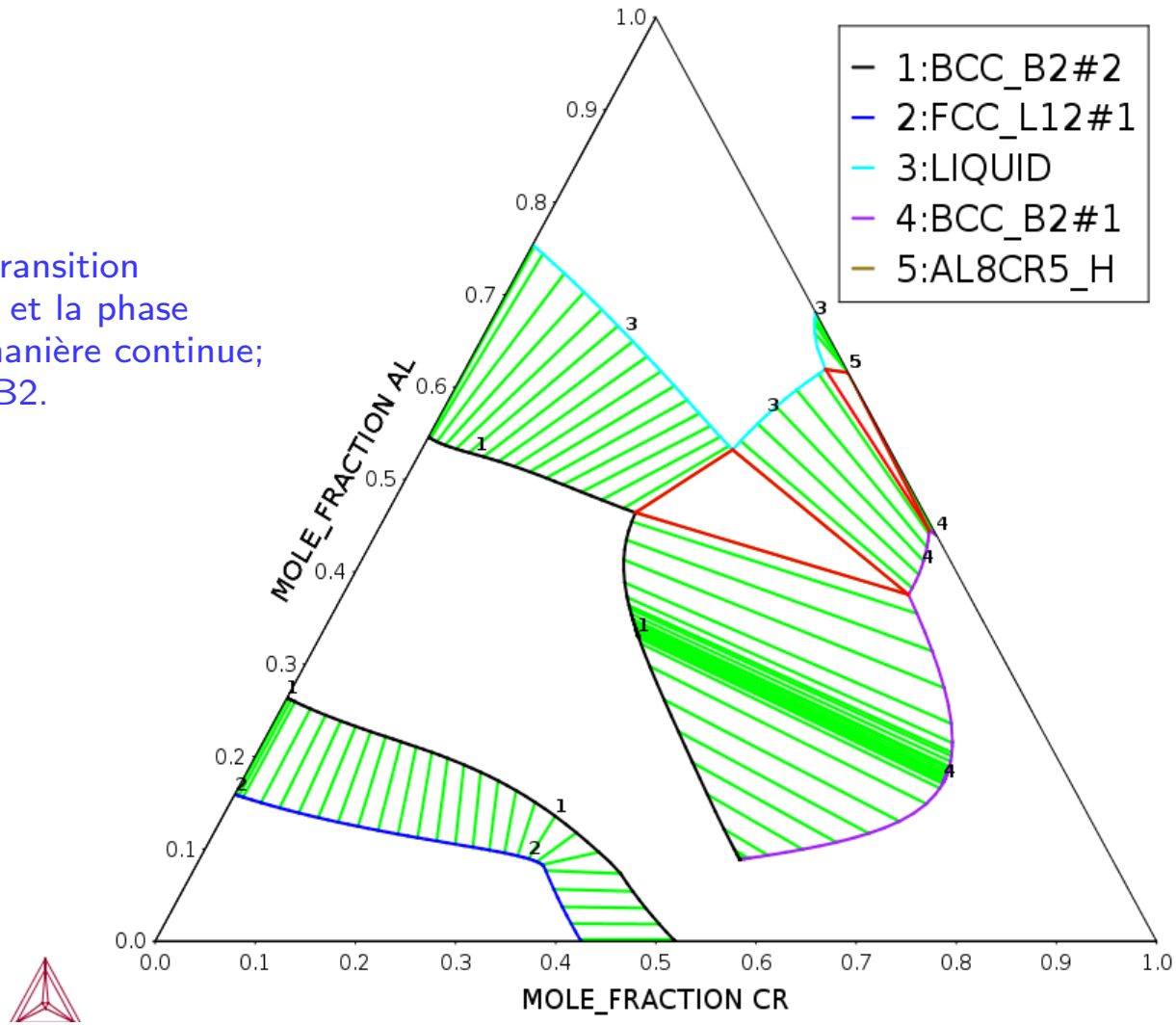


Al-Co-Cr à 1300 °C

```
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.



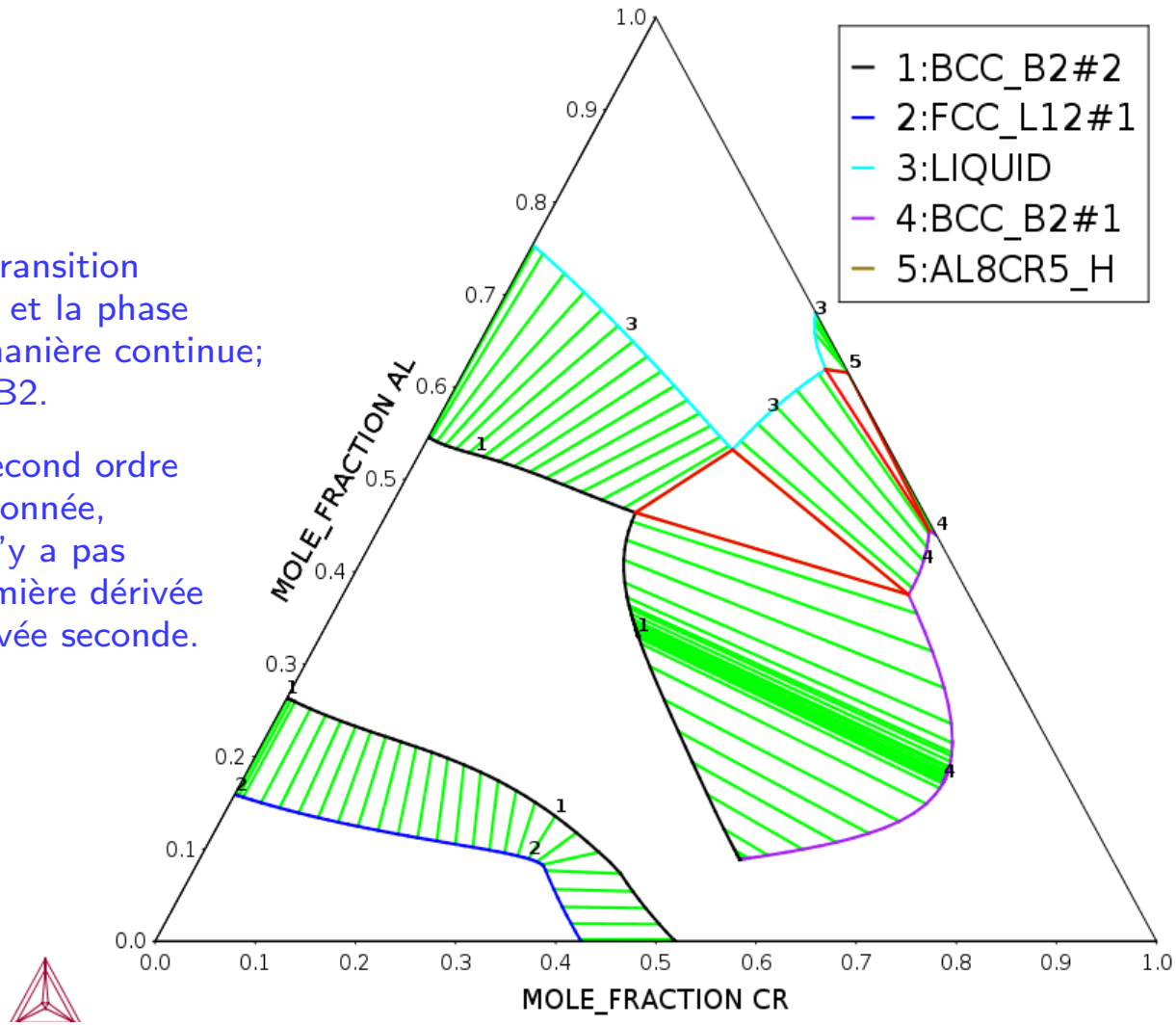
Al-Co-Cr à 1300 °C

```
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.



Al-Co-Cr à 1300 °C

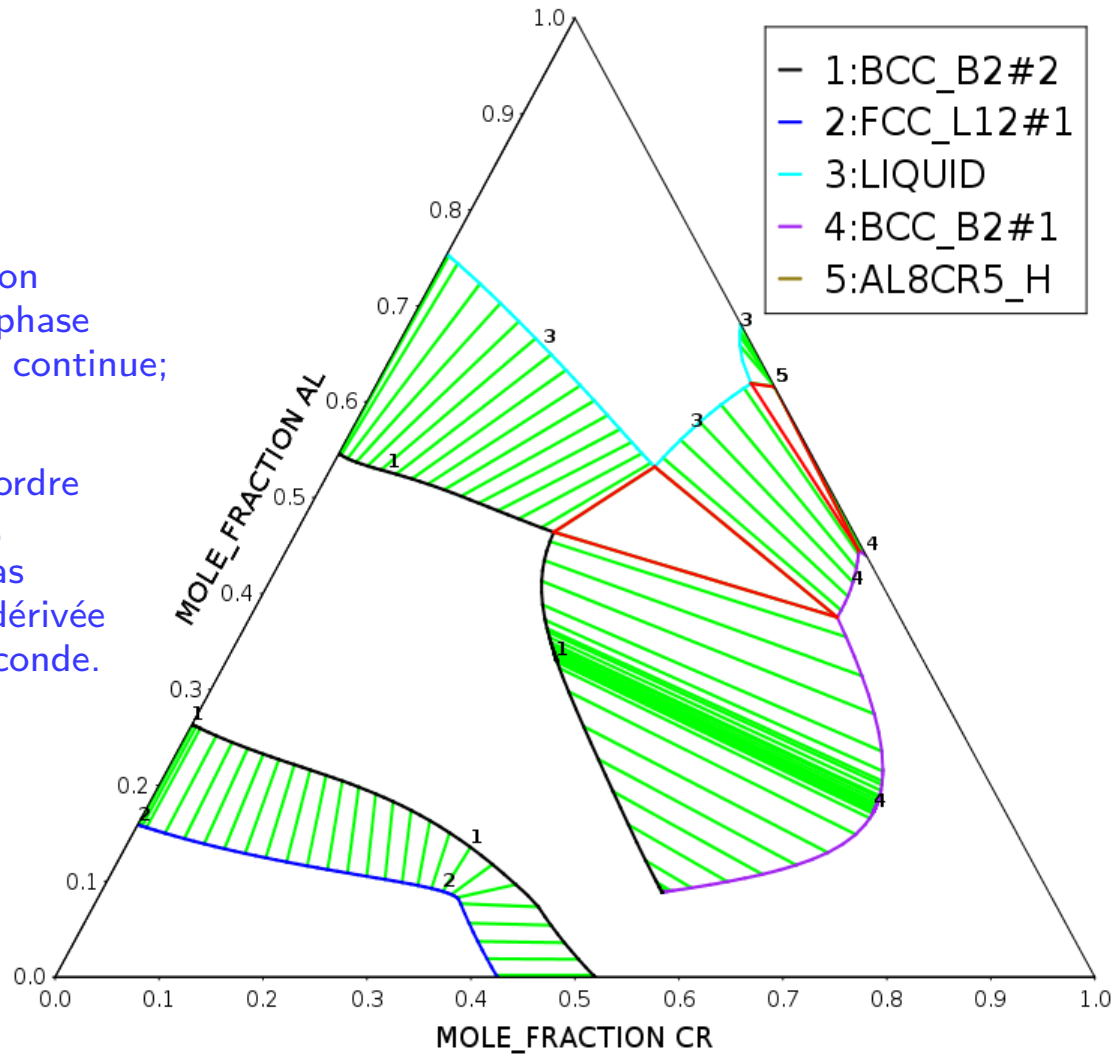
```
go ter
TCNI
Co Cr Al

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.

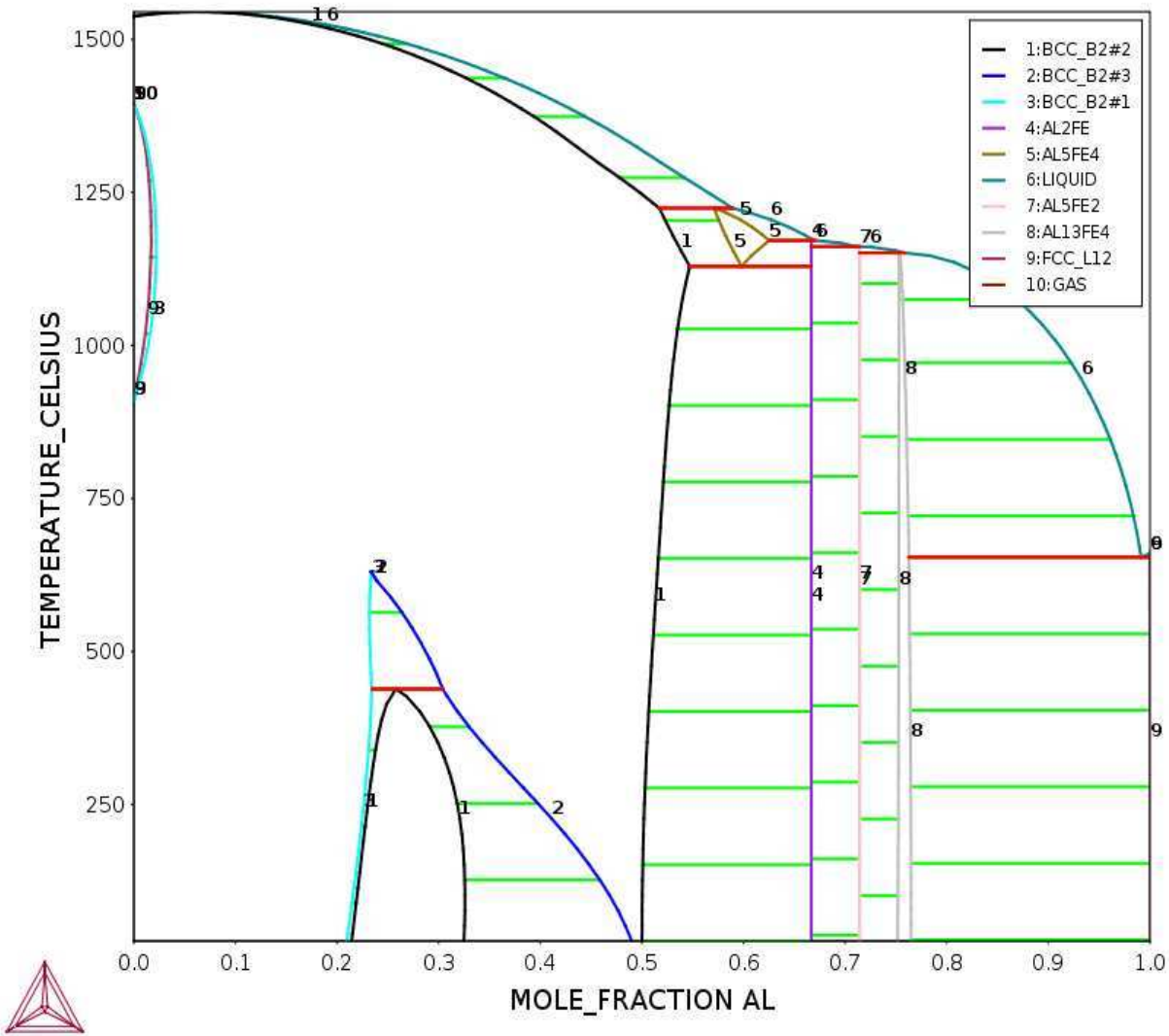


Al-Fe (tcex16)

```
set_log alfe
transition de 2nd ordre
go bin
TCNI
Fe Al
```

Al-Fe (tcex16)

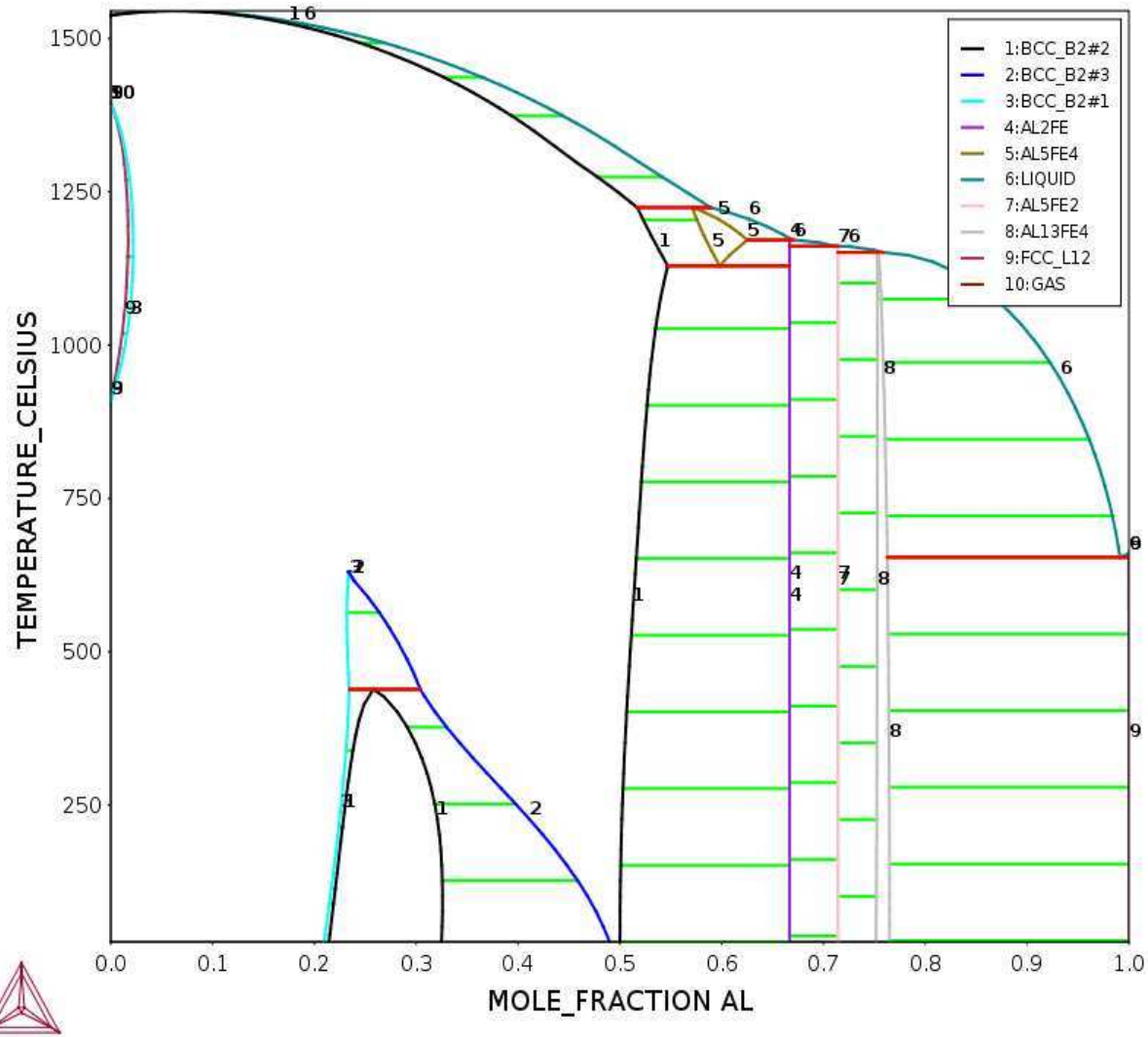
```
set_log alfe
transition de 2nd ordre
go bin
TCNI
Fe Al
```



Al-Fe (tcex16)

```
set_log alfe
transition de 2nd ordre
go bin
TCNI
Fe Al
```

Il existe un domaine dans lequel la transition B2/A2 est de second ordre.

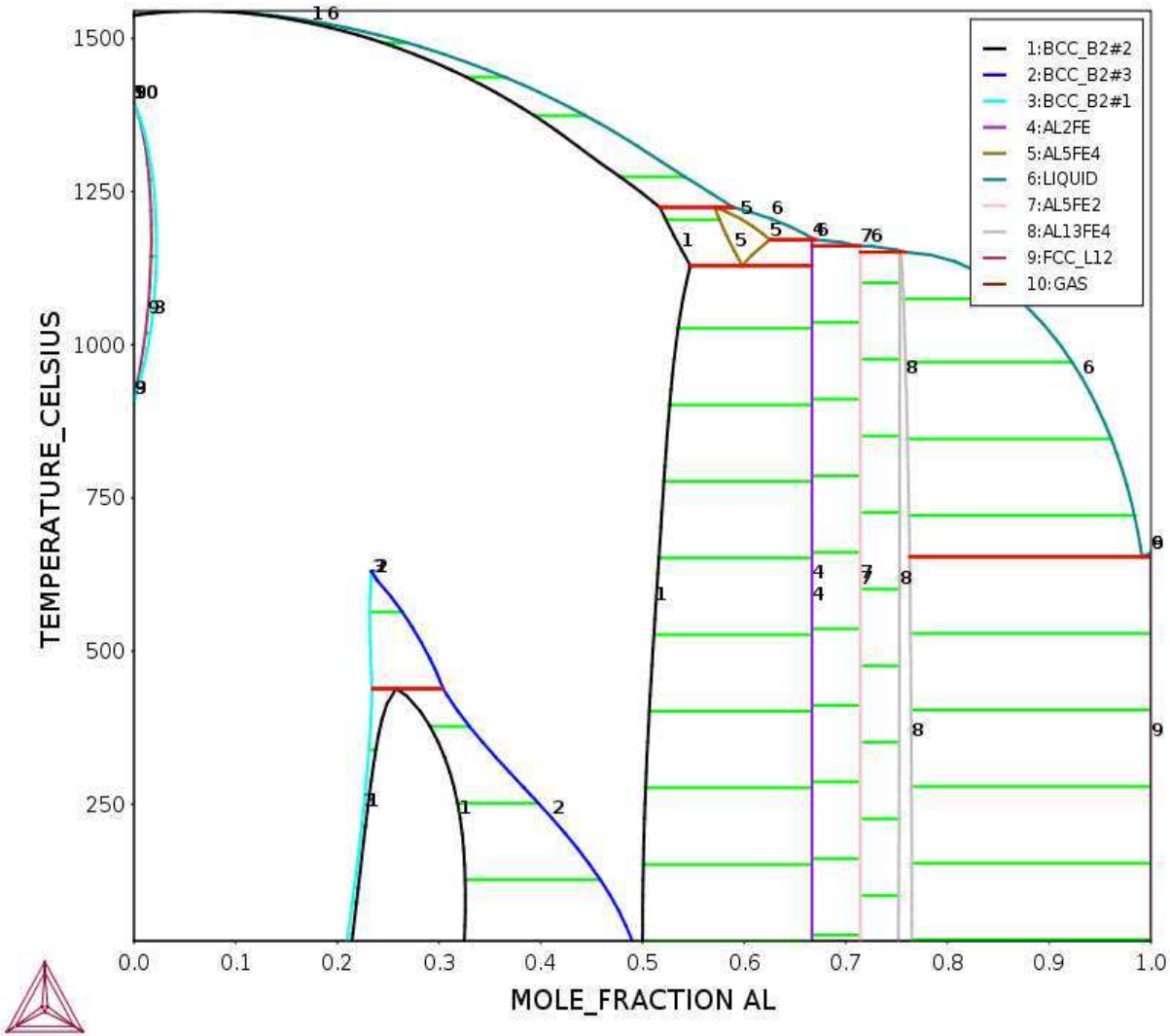


Al-Fe (tcex16)

```
set_log alfe
transition de 2nd ordre
go bin
TCNI
Fe Al
```

Il existe un domaine dans lequel la transition B2/A2 est de second ordre.

Son tracé nécessite un autre calcul et une connaissance un peu plus poussée de TC.



2nd ordre

Afin de tracer une ligne de transition du second ordre, il faut :

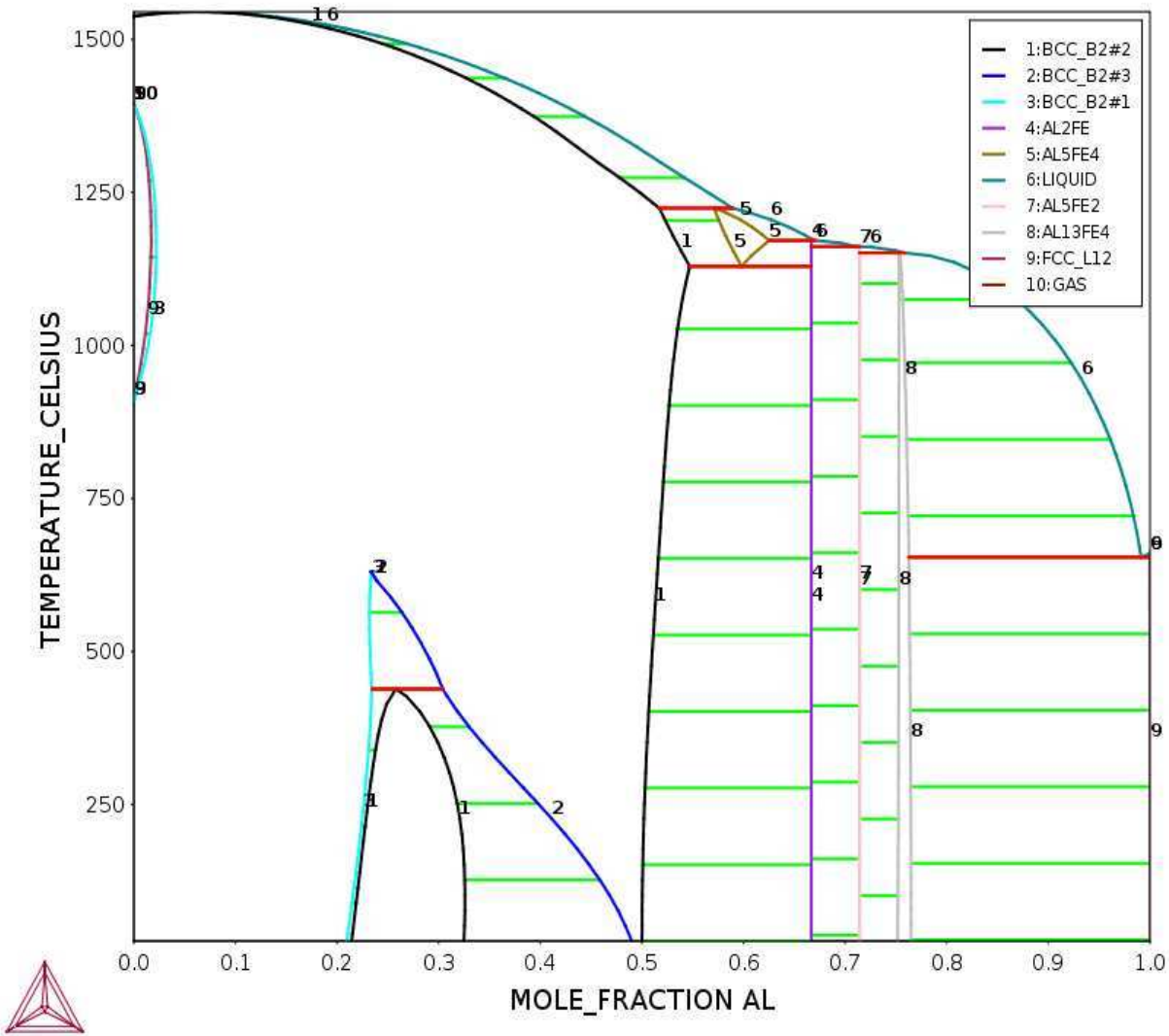
- ne considérer que la phase concernée,
- calculer un équilibre monophasé dans le domaine ordonné,
- empêcher la `global minimisation`,
- remplacer l'une des conditions habituelles par une contrainte sur le degré d'ordre,
- calculer l'équilibre contraint,
- enlever l'axe correspondant à la condition remplacée,
- calculer en incrémentant l'axe restant (step),
- représenter graphiquement le résultat.

Al-Fe

```
set_log alfe
transition de 2nd ordre
go bin
TCNI
Fe Al

b
go pol
l_c
rea,,
ch_st p *=s
ch_st p bcc_b=e 1
s_c t=1000 x(fe)=.7
c_e
l_e

N
l_st p
adv glo n n
```



Al-Fe

```
set_log alfe
transition de 2nd ordre
go bin
TCNI
Fe Al

b
go pol
l_c
rea,,
ch_st p *=s
ch_st p bcc_b=e 1
s_c t=1000 x(fe)=.7
c_e
l_e

N
l_st p
adv glo n n
```

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

 Conditions:
 X(FE)=0.7, P=1E5, N=1, T=1000
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  4.71875E+01
 Total Gibbs energy -6.47936E+04,  Enthalpy  1.45710E+03,  Volume  7.62126E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      3.0000E-01  1.7154E-01 1.7292E-03 -5.2881E+04 FCC_A1
 FE                      7.0000E-01  8.2846E-01 3.1281E-01 -9.6627E+03 BCC_A2#1

 BCC_B2#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.7188E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  8.28459E-01  AL  1.71541E-01
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 FE  9.46413E-01  AL  5.35870E-02  VA  6.09422E-09
 Sublattice  2,  Number of sites  5.0000E-01
 AL  5.46413E-01  FE  4.53587E-01  VA  5.18450E-08
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY_3:l_st p
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 BCC_B2#2                ENTERED      0.000000E+00    1.000000E+00
 SUSPENDED PHASES:
 SIGMA NI3TI_D024 NI3TA_D0A MU_PHASE HCP_A3 HALITE FCC_L12 DIAMOND_A4 CUB_A13
 CHI_A12 CBCC_A12 C14_LAVES BCT_D022 BCC_B2#3 BCC_B2#1 AL5FE4 AL5FE2 AL2FE
 AL13FE4 LIQUID GAS
```

Al-Fe

```
set_log alfe
transition de 2nd ordre
go bin
TCNI
Fe Al

b
go pol
l_c
rea,,
ch_st p *=s
ch_st p bcc_b=e 1
s_c t=1000 x(fe)=.7
c_e
l_e

N
l_st p
adv glo n n
```

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

 Conditions:
 X(FE)=0.7, P=1E5, N=1, T=1000
 DEGREES OF FREEDOM 0

 Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
 Number of moles of components  1.00000E+00,  Mass in grams  4.71875E+01
 Total Gibbs energy -6.47936E+04,  Enthalpy  1.45710E+03,  Volume  7.62126E-06

 Component               Moles       W-Fraction  Activity   Potential  Ref.stat
 AL                      3.0000E-01  1.7154E-01 1.7292E-03 -5.2881E+04 FCC_A1
 FE                      7.0000E-01  8.2846E-01 3.1281E-01 -9.6627E+03 BCC_A2#1

 BCC_B2#2                    Status ENTERED     Driving force  0.0000E+00
 Moles 1.0000E+00, Mass 4.7188E+01, Volume fraction 1.0000E+00  Mass fractions:
 FE  8.28459E-01  AL  1.71541E-01
 Constitution:
 Sublattice  1,  Number of sites  5.0000E-01
 FE  9.46413E-01  AL  5.35870E-02  VA  6.09422E-09
 Sublattice  2,  Number of sites  5.0000E-01
 AL  5.46413E-01  FE  4.53587E-01  VA  5.18450E-08
 Sublattice  3,  Number of sites  3.0000E+00
 VA  1.00000E+00
POLY_3:l_st p
 *** STATUS FOR ALL PHASES
 PHASE                   STATUS    DRIVING FORCE   MOLES
 BCC_B2#2                ENTERED      0.000000E+00    1.000000E+00
 SUSPENDED PHASES:
 SIGMA NI3TI_D024 NI3TA_D0A MU_PHASE HCP_A3 HALITE FCC_L12 DIAMOND_A4 CUB_A13
 CHI_A12 CBCC_A12 C14_LAVES BCT_D022 BCC_B2#3 BCC_B2#1 AL5FE4 AL5FE2 AL2FE
 AL13FE4 LIQUID GAS
```

La phase ENTERED, initialement BCC_B2#1, a été remplacée par POLY_3 sans avertissement.

Al-Fe

```
BCC_B2#2                    Status ENTERED     Driving force  0.0000E+00
Moles 1.0000E+00, Mass 4.7188E+01, Volume fraction 1.0000E+00  Mass fractions:
FE  8.28459E-01  AL  1.71541E-01
Constitution:
Sublattice  1,  Number of sites  5.0000E-01
FE  9.46413E-01  AL  5.35870E-02  VA  6.09422E-09
Sublattice  2,  Number of sites  5.0000E-01
AL  5.46413E-01  FE  4.53587E-01  VA  5.18450E-08
Sublattice  3,  Number of sites  3.0000E+00
VA  1.00000E+00
```

```
s_c x(fe)=none y(bcc_b2#2,fe)-y(bcc_b2#2,fe#2)=.1
c_e
l_e
```

Al-Fe

```
BCC_B2#2                    Status ENTERED     Driving force  0.0000E+00
Moles 1.0000E+00, Mass 4.7188E+01, Volume fraction 1.0000E+00  Mass fractions:
FE  8.28459E-01  AL  1.71541E-01
Constitution:
Sublattice  1,  Number of sites  5.0000E-01
FE  9.46413E-01  AL  5.35870E-02  VA  6.09422E-09
Sublattice  2,  Number of sites  5.0000E-01
AL  5.46413E-01  FE  4.53587E-01  VA  5.18450E-08
Sublattice  3,  Number of sites  3.0000E+00
VA  1.00000E+00
```

```
s_c x(fe)=none y(bcc_b2#2,fe)-y(bcc_b2#2,fe#2)=.1
c_e
l_e
```

La contrainte introduite tient compte de l'équilibre courant.
Il faut prendre garde de l'exprimer pour la phase courante,
ici BCC_B2#2, et avec des fractions d'occupation proches
cad, pour cet exemple, plus de Fe dans le premier
sous-réseau que dans le deuxième.

Al-Fe

```
BCC_B2#2                    Status ENTERED     Driving force  0.0000E+00
Moles 1.0000E+00, Mass 4.7188E+01, Volume fraction 1.0000E+00  Mass fractions:
FE  8.28459E-01  AL  1.71541E-01
Constitution:
Sublattice  1,  Number of sites  5.0000E-01
FE  9.46413E-01  AL  5.35870E-02  VA  6.09422E-09
Sublattice  2,  Number of sites  5.0000E-01
AL  5.46413E-01  FE  4.53587E-01  VA  5.18450E-08
Sublattice  3,  Number of sites  3.0000E+00
VA  1.00000E+00
```

```
s_c x(fe)=none y(bcc_b2#2,fe)-y(bcc_b2#2,fe#2)=.1
c_e
l_e
```

```
Conditions:
P=1E5, N=1, T=1000, Y(BCC_B2#2,FE)-Y(BCC_B2#2,FE#2)=0.1
DEGREES OF FREEDOM 0

Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
Number of moles of components  1.00000E+00,  Mass in grams  4.88049E+01
Total Gibbs energy -6.22201E+04,  Enthalpy  5.31965E+03,  Volume  7.68146E-06

Component               Moles       W-Fraction  Activity   Potential  Ref.stat
AL                      2.4397E-01  1.3488E-01 1.0397E-03 -5.7111E+04 FCC_A1
FE                      7.5603E-01  8.6512E-01 3.7884E-01 -8.0704E+03 BCC_A2#1

BCC_B2#2                    Status ENTERED     Driving force  0.0000E+00
Moles 1.0000E+00, Mass 4.8805E+01, Volume fraction 1.0000E+00  Mass fractions:
FE  8.65121E-01  AL  1.34879E-01
Constitution:
Sublattice  1,  Number of sites  5.0000E-01
FE  8.06032E-01  AL  1.93968E-01  VA  1.03005E-08
Sublattice  2,  Number of sites  5.0000E-01
FE  7.06032E-01  AL  2.93968E-01  VA  1.59456E-08
Sublattice  3,  Number of sites  3.0000E+00
VA  1.00000E+00
```

Al-Fe

```
Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
Number of moles of components  1.00000E+00,  Mass in grams  4.88049E+01
Total Gibbs energy -6.22201E+04,  Enthalpy  5.31965E+03,  Volume  7.68146E-06

Component               Moles       W-Fraction  Activity   Potential  Ref.stat
AL                      2.4397E-01  1.3488E-01 1.0397E-03 -5.7111E+04 FCC_A1
FE                      7.5603E-01  8.6512E-01 3.7884E-01 -8.0704E+03 BCC_A2#1

BCC_B2#2                    Status ENTERED     Driving force  0.0000E+00
Moles 1.0000E+00, Mass 4.8805E+01, Volume fraction 1.0000E+00  Mass fractions:
FE  8.65121E-01  AL  1.34879E-01
Constitution:
Sublattice  1,  Number of sites  5.0000E-01
FE  8.06032E-01  AL  1.93968E-01  VA  1.03005E-08
Sublattice  2,  Number of sites  5.0000E-01
FE  7.06032E-01  AL  2.93968E-01  VA  1.59456E-08
Sublattice  3,  Number of sites  3.0000E+00
VA  1.00000E+00
```

```
s_c y(bcc_b2#2,fe)-y(bcc_b2#2,fe#2)=1e-4
c_e
l_e
```

Al-Fe

```
Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
Number of moles of components  1.00000E+00,  Mass in grams  4.88049E+01
Total Gibbs energy -6.22201E+04,  Enthalpy  5.31965E+03,  Volume  7.68146E-06

Component               Moles       W-Fraction  Activity   Potential  Ref.stat
AL                      2.4397E-01  1.3488E-01 1.0397E-03 -5.7111E+04 FCC_A1
FE                      7.5603E-01  8.6512E-01 3.7884E-01 -8.0704E+03 BCC_A2#1

BCC_B2#2                    Status ENTERED     Driving force  0.0000E+00
Moles 1.0000E+00, Mass 4.8805E+01, Volume fraction 1.0000E+00  Mass fractions:
FE  8.65121E-01  AL  1.34879E-01
Constitution:
Sublattice  1,  Number of sites  5.0000E-01
FE  8.06032E-01  AL  1.93968E-01  VA  1.03005E-08
Sublattice  2,  Number of sites  5.0000E-01
FE  7.06032E-01  AL  2.93968E-01  VA  1.59456E-08
Sublattice  3,  Number of sites  3.0000E+00
VA  1.00000E+00
```

```
s_c y(bcc_b2#2,fe)-y(bcc_b2#2,fe#2)=1e-4
c_e
l_e
```

```
Temperature   1000.00 K (   726.85 C),  Pressure  1.000000E+05
Number of moles of components  1.00000E+00,  Mass in grams  4.88623E+01
Total Gibbs energy -6.21231E+04,  Enthalpy  5.45289E+03,  Volume  7.68560E-06

Component               Moles       W-Fraction  Activity   Potential  Ref.stat
AL                      2.4198E-01  1.3362E-01 1.0243E-03 -5.7235E+04 FCC_A1
FE                      7.5802E-01  8.6638E-01 3.8066E-01 -8.0306E+03 BCC_A2#1

BCC_B2#2                    Status ENTERED     Driving force  0.0000E+00
Moles 1.0000E+00, Mass 4.8862E+01, Volume fraction 1.0000E+00  Mass fractions:
FE  8.66378E-01  AL  1.33622E-01
Constitution:
Sublattice  1,  Number of sites  5.0000E-01
FE  7.58070E-01  AL  2.41930E-01  VA  1.26291E-08
Sublattice  2,  Number of sites  5.0000E-01
FE  7.57970E-01  AL  2.42030E-01  VA  1.26347E-08
Sublattice  3,  Number of sites  3.0000E+00
VA  1.00000E+00
```

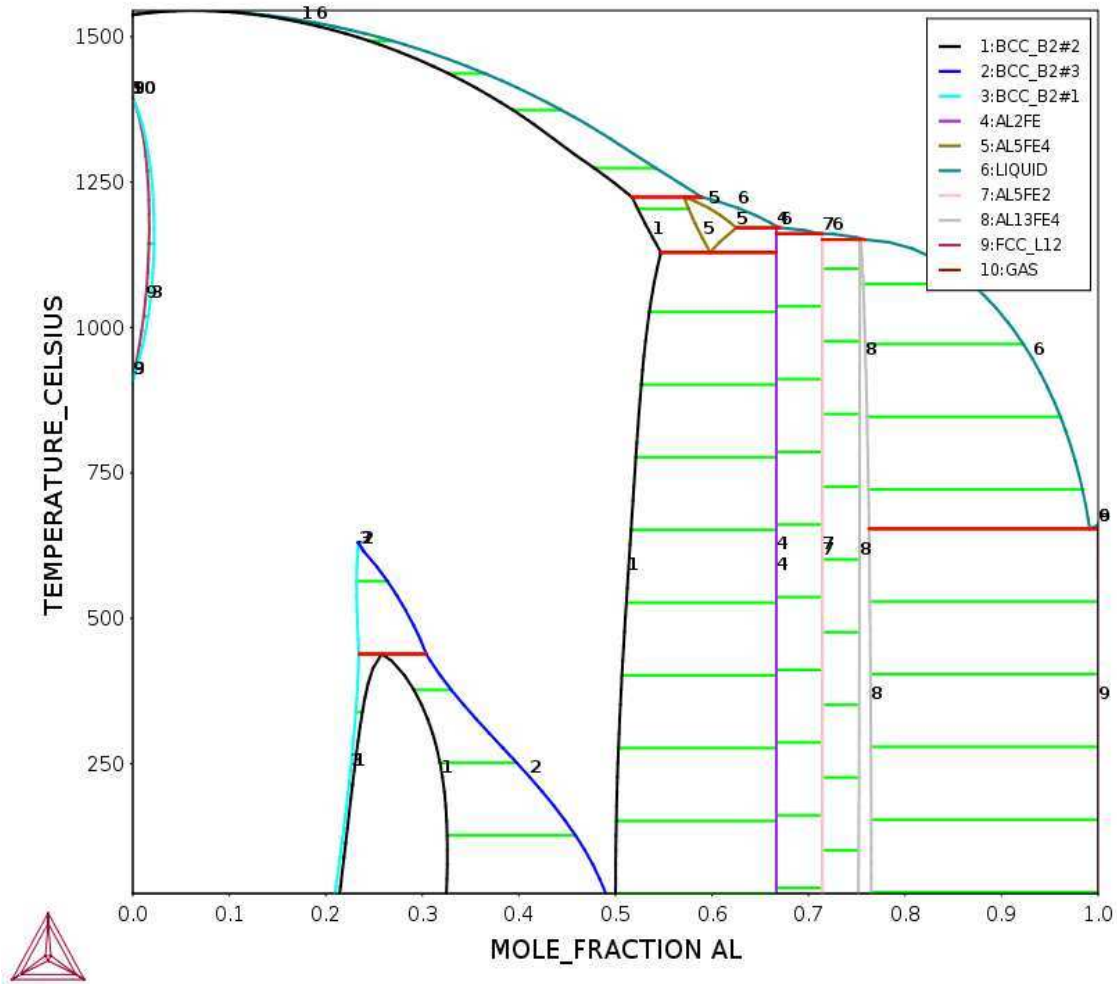
Al-Fe

```
l-a-v
s_a_v 2 none
s_a_v 1 t 900 1576

li-i
del_i

step

po
pl
```



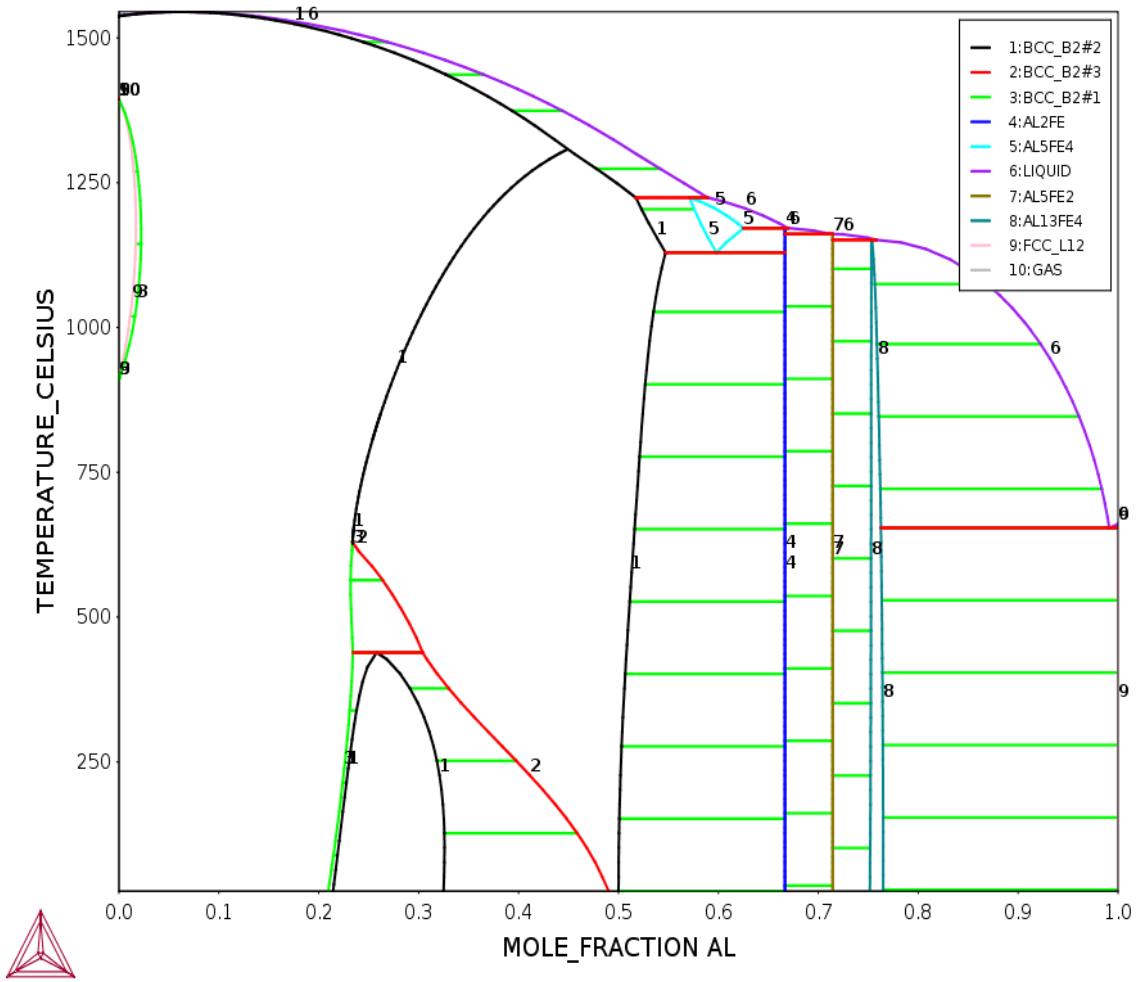
Al-Fe

```
l-a-v
s_a_v 2 none
s_a_v 1 t 900 1576

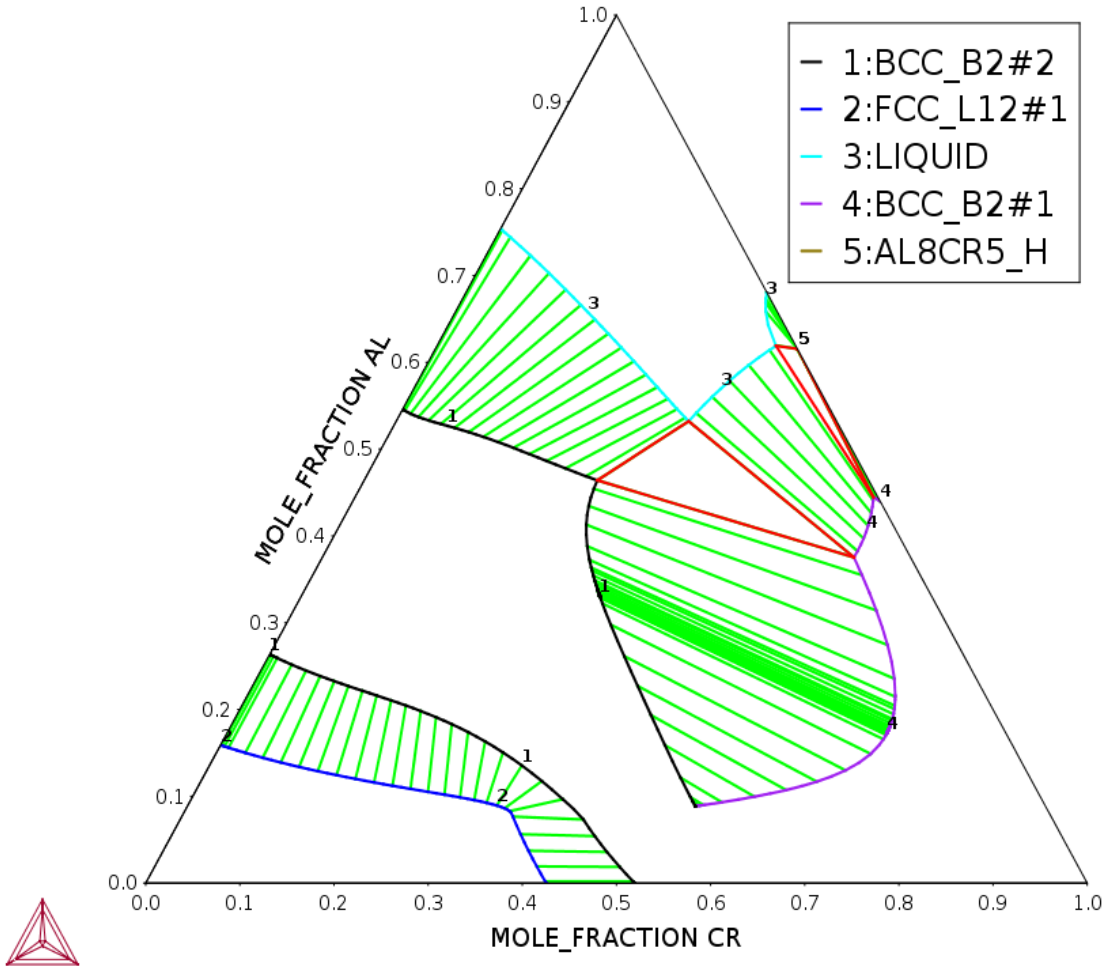
li-i
del_i

step

po
pl
```



Al-Co-Cr à 1300 °C



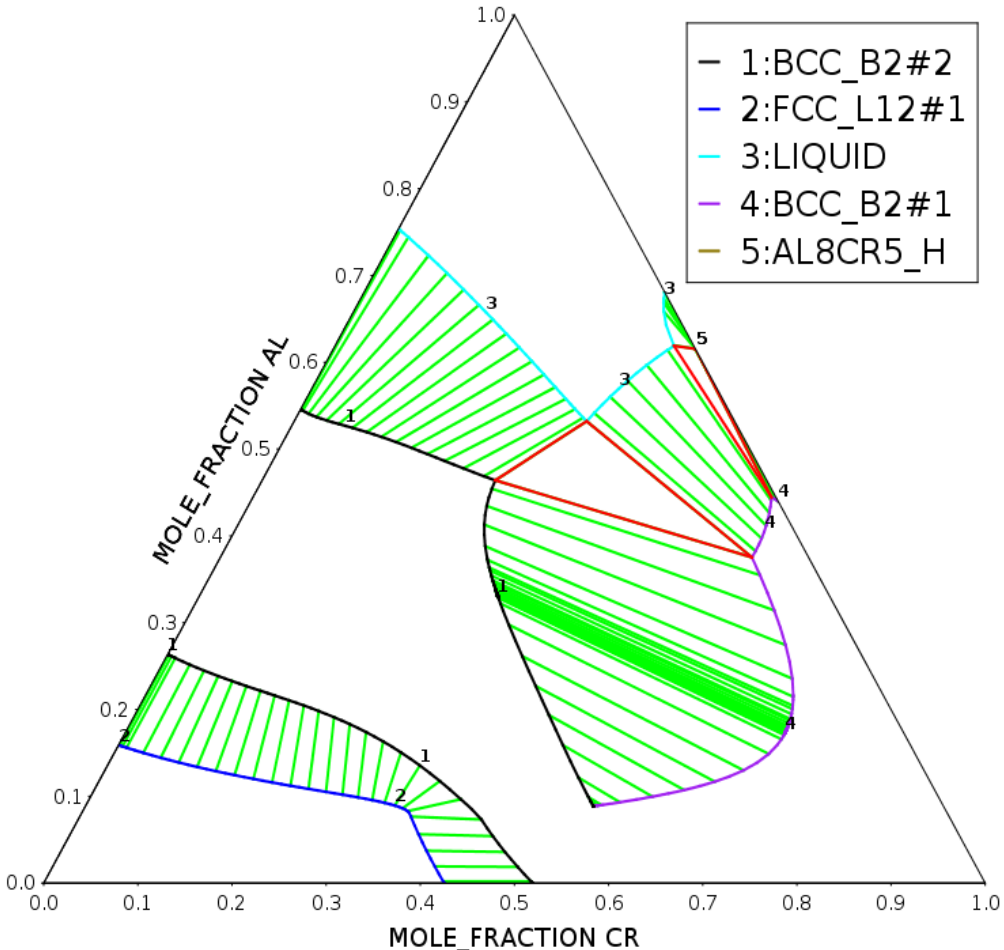
Al-Co-Cr à 1300 °C

```
set_log alcocr
transition du 2nd ordre
go ter
TCNI
Co Cr Al

1300

b
go pol
l_c
rea,,
s_c x(co)=.4 x(cr)=.5
c_e
l_e

N
ch_st p *=s
ch_st p bcc_b#2=e 1
adv glo n n
s_c x(co)=none
s_c y(bcc_b2#2,co)-y(bcc_b2#2,co#2)=.1
c_e
l_e
```



Al-Co-Cr à 1300 °C

```
set_log alcocr
transition du 2nd ordre
go ter
TCNI
Co Cr Al

1300

b
go pol
l_c
rea,,
s_c x(co)=.4 x(cr)=.5
c_e
l_e

N
ch_st p *=s
ch_st p bcc_b#2=e 1
adv glo n n
s_c x(co)=none
s_c y(bcc_b2#2,co)-y(bcc_b2#2,co#2)=.1
c_e
l_e
s_c y(bcc_b2#2,co)-y(bcc_b2#2,co#2)=1e-4
c_e
l_e


l-a-v
s_a_v 2 none
s_a_v 1 x(cr) .43 .54

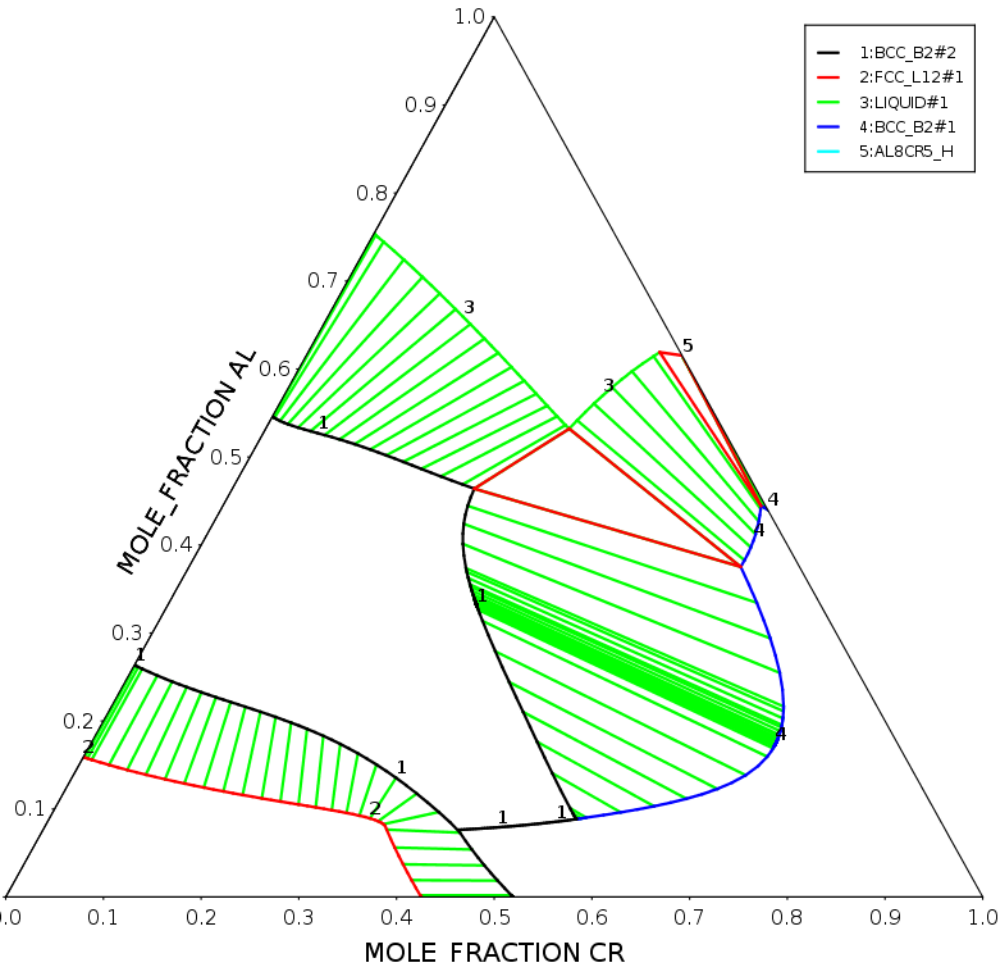
li-i
del_i

step

po
pl
```

Al-Co-Cr à 1300 °C

```
set_log alcocr
transition du 2nd ordre
```




```
s_c y(bcc_b2#2,co)-y(bcc_b2#2,co#2)=1e-4
c_e
l_e


l-a-v
s_a_v 2 none
s_a_v 1 x(cr) .43 .54

li-i
del_i

step

po
pl
```

Al-Co-Cr à 1400 °C

Al-Co-Cr à 1400 °C

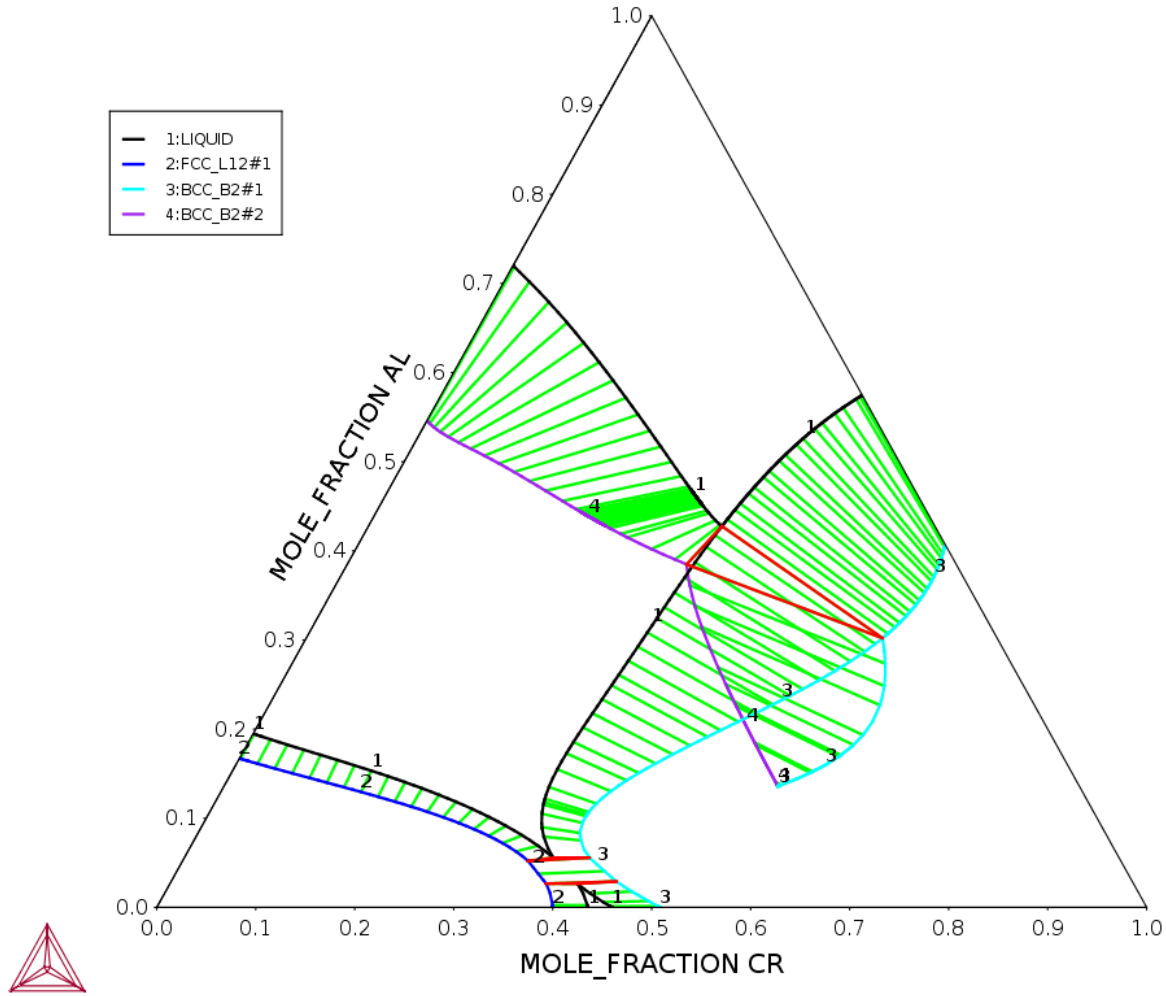
```
set_log alcocr1400
calcul metastable
go ter
TCNI
Co Cr Al

1400
```

Al-Co-Cr à 1400 °C

```
set_log alcocr1400
calcul metastable
go ter
TCNI
Co Cr Al

1400
```



Les modules BINARY et TERNARY permettent de restaurer les phases stables dans le système considéré mais rejetées par défaut pour les calculs d'alliages complexes.
Ils n'empêchent pas l'obtention de calculs métastables.
Un nouveau calcul avec un point de départ plus adapté peut être nécessaire pour obtenir un diagramme de phase exempt de domaine métastable.

Al-Co-Cr à 1400 °C

```
set_log alcocr1400
calcul metastable
go ter
TCNI
Co Cr Al

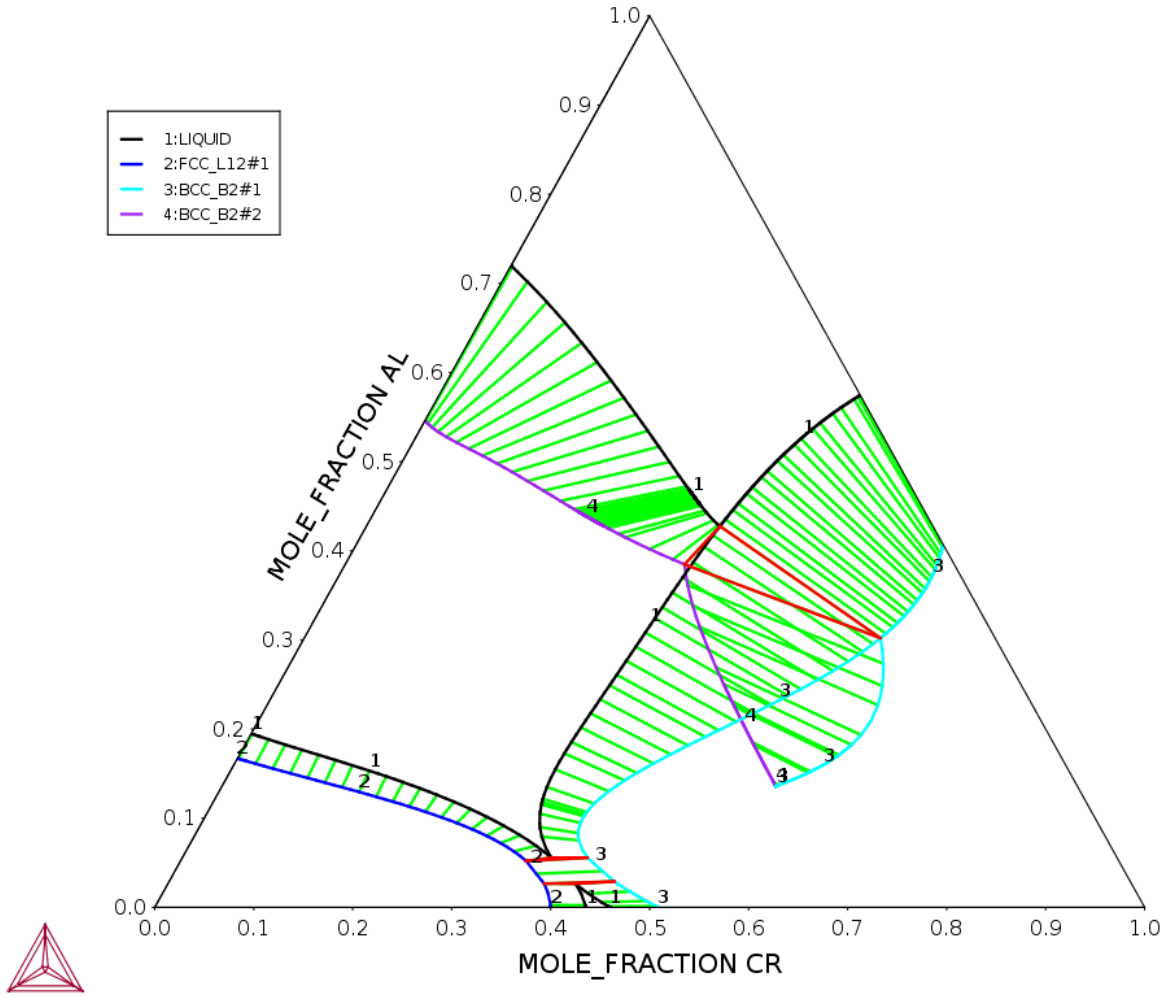
1400



b
go pol
l_c
rea,,
s_c x(co)=.2 x(cr)=.5
c_e
l_e

N
li_i
del_i

sa alcocr1400 y
add 1
map
po
pl
```



Les modules BINARY et TERNARY permettent de restaurer les phases stables dans le système considéré mais rejetées par défaut pour les calculs d'alliages complexes.
Ils n'empêchent pas l'obtention de calculs métastables.
Un nouveau calcul avec un point de départ plus adapté peut être nécessaire pour obtenir un diagramme de phase exempt de domaine métastable.

Al-Co-Cr à 1400 °C

```
set_log alcocr1400
calcul metastable
go ter
TCNI
Co Cr Al

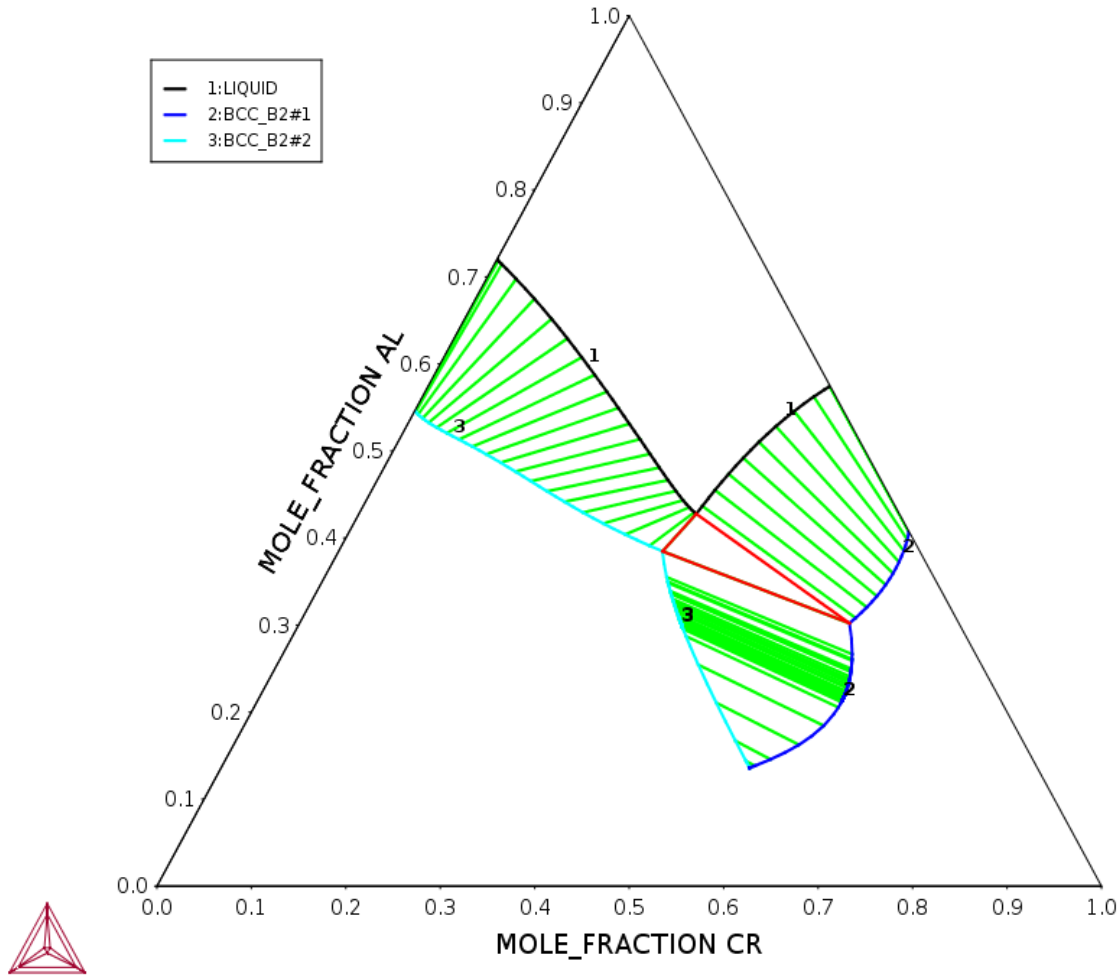
1400



b
go pol
l_c
rea,,
s_c x(co)=.2 x(cr)=.5
c_e
l_e

N
li_i
del_i

sa alcocr1400 y
add 1
map
po
pl
```



Le domaine métastable a disparu mais aussi les équilibres impliquant la phase fcc dans le coin riche en Co.
Un autre point de départ est nécessaire.

Al-Co-Cr à 1400 °C

```
set_log alcocr1400
calcul metastable
go ter
TCNI
Co Cr Al

1400



b
go pol
l_c
rea,,
s_c x(co)=.2 x(cr)=.5
c_e
l_e

N
li_i
del_i

sa alcocr1400 y
add 1
map
po
pl
```

```
b
l_c
s_c x(co)=.7 x(cr)=.1
c_e
l_e,,,
l_a_v
add 2
map
po
pl
```

Al-Co-Cr à 1400 °C

```
set_log alcocr1400
calcul metastable
go ter
TCNI
Co Cr Al

1400

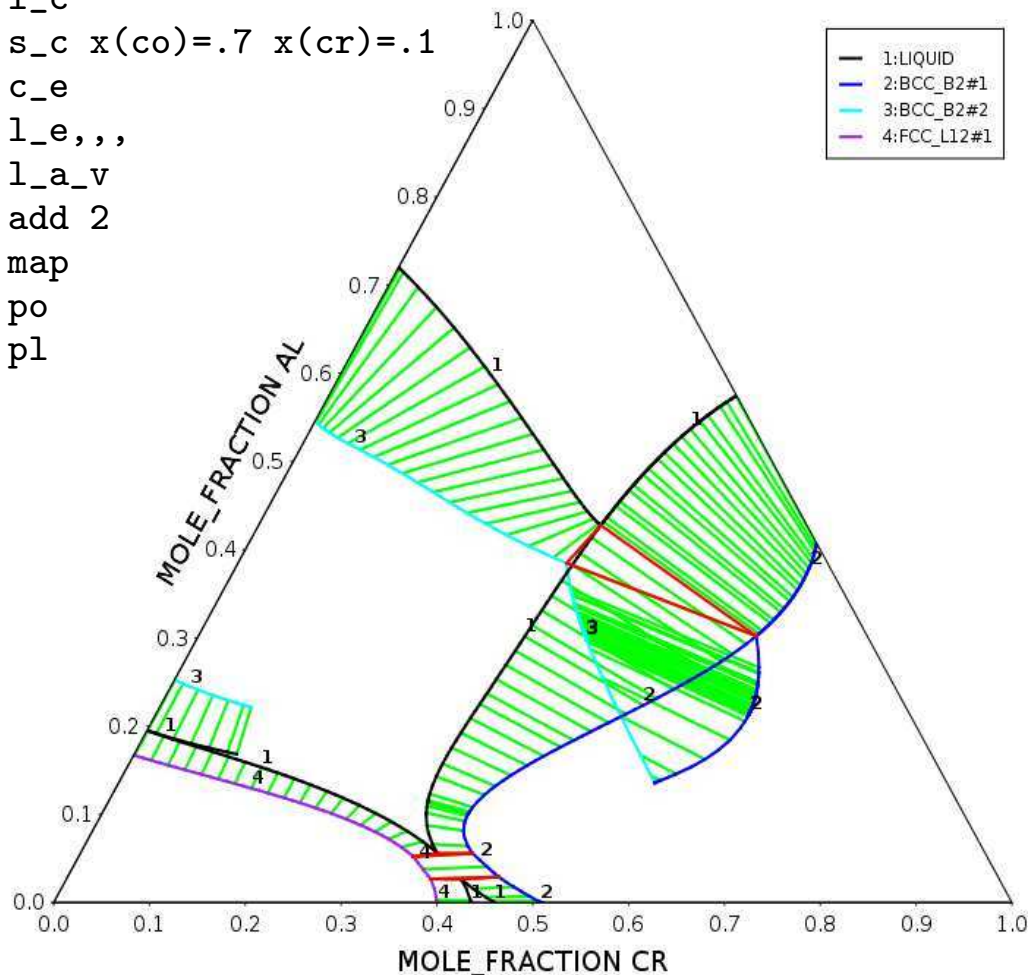


b
go pol
l_c
rea,,
s_c x(co)=.2 x(cr)=.5
c_e
l_e

N
li_i
del_i

sa alcocr1400 y
add 1
map
po
pl
```

```
b
l_c
s_c x(co)=.7 x(cr)=.1
c_e
l_e,,,
l_a_v
add 2
map
po
pl
```



Retour des équilibres métastables!
Il faut faire des tests avec `global minimisation` plus souvent.

Al-Co-Cr à 1400 °C

```
set_log alcocr1400
calcul metastable
go ter
TCNI
Co Cr Al

1400



b
go pol
l_c
rea,,
s_c x(co)=.2 x(cr)=.5
c_e
l_e

N
li_i
del_i

sa alcocr1400 y
add 1
map
po
pl
```

```
b
l_c
s_c x(co)=.7 x(cr)=.1
c_e
l_e,,,
l_a_v
add 2
map
po
pl

b
rea,,
sa,, y
add 1
s_c x(co)=.7 x(cr)=.1
c_e
adv

1
N
add 1
map
po
pl
```

Al-Co-Cr à 1400 °C

```
set_log alcocr1400
calcul metastable
go ter
TCNI
Co Cr Al

1400



b
go pol
l_c
rea,,
s_c x(co)=.2 x(cr)=.5
c_e
l_e

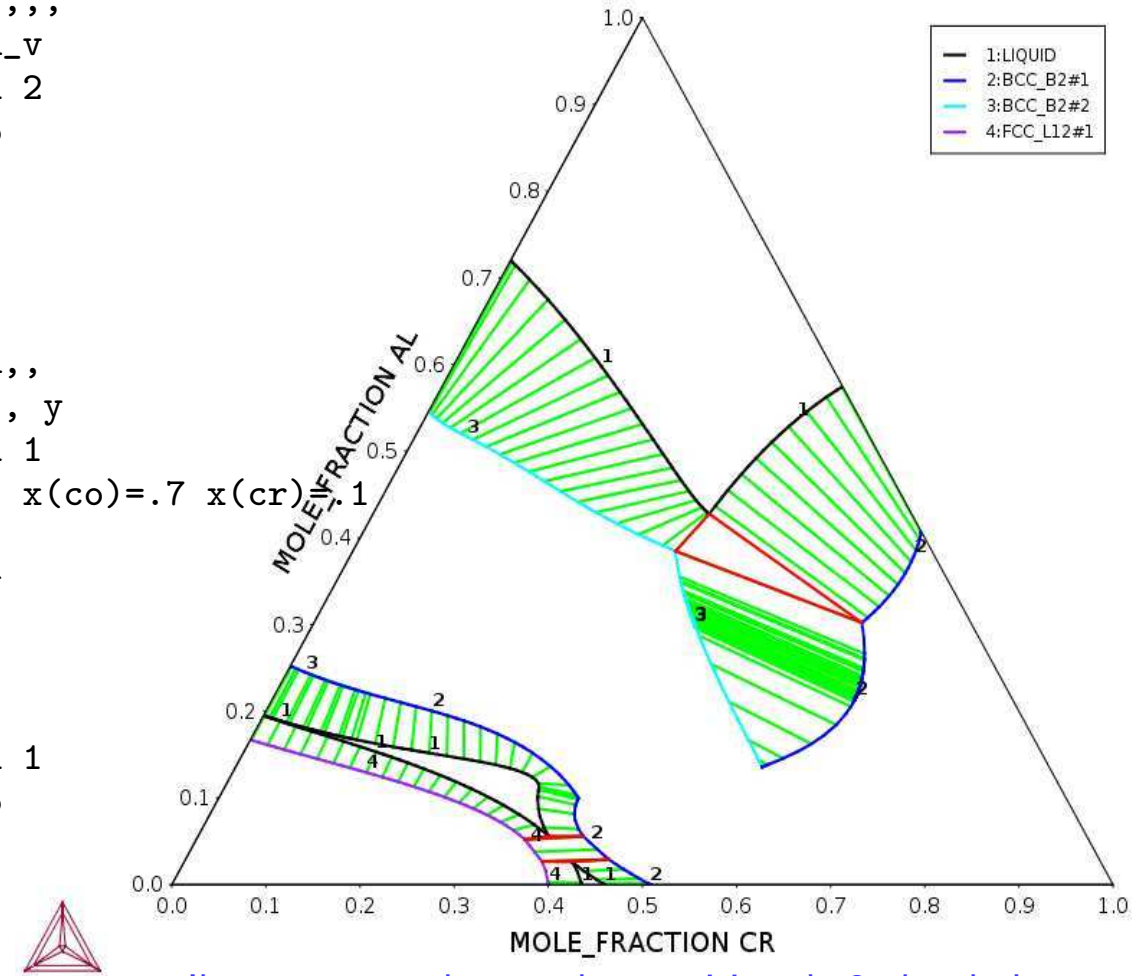
N
li_i
del_i

sa alcocr1400 y
add 1
map
po
pl
```

```
b
l_c
s_c x(co)=.7 x(cr)=.1
c_e
l_e,,,
l_a_v
add 2
map
po
pl

b
rea,,
sa,, y
add 1
s_c x(co)=.7 x(cr)=.1
c_e
adv

1
N
add 1
map
po
pl
```



Il ne manque plus que la transition de 2nd ordre!

Al-Co-Cr à 1400 °C

```
set_log alcocr1400
calcul metastable
go ter
TCNI
Co Cr Al

1400



b
go pol
l_c
rea,,
s_c x(co)=.2 x(cr)=.5
c_e
l_e

N
li_i
del_i

sa alcocr1400 y
add 1
map
po
pl
```

```
b
l_c
s_c x(co)=.7 x(cr)=.1
c_e
l_e,,,
l_a_v
add 2
map
po
pl

b
rea,,
sa,, y
add 1
s_c x(co)=.7 x(cr)=.1
c_e
adv

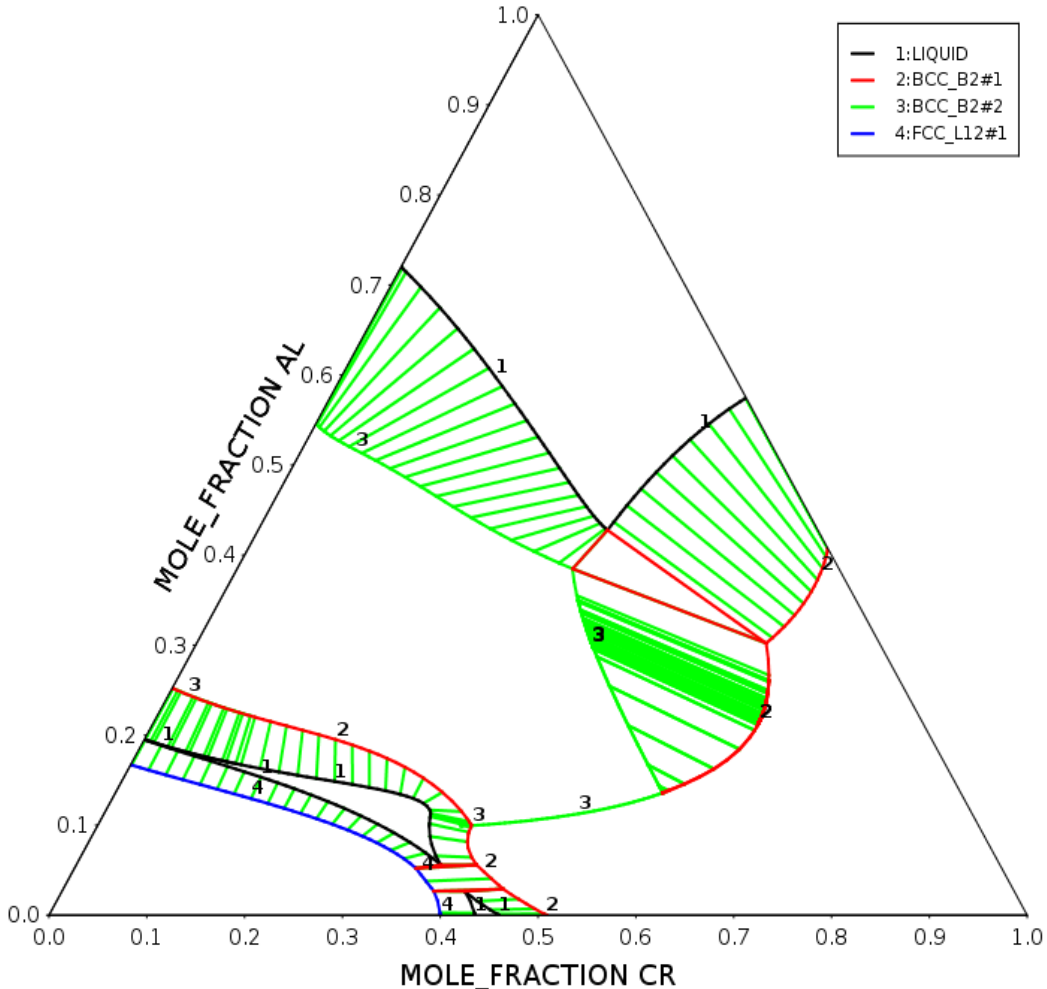
1
N
add 1
map
po
pl
```

```
b
l_c
s_c x(co)=.5 x(cr)=.3
c_e
l_e,,,
ch_st p *=s
ch_st p bcc_b#2=e 1
adv glo n n
s_c x(cr)=none
s_c y(b_b#2,co)-y(b_b#2,co#2)=.1
c_e
l_e,,,
s_c y(b_b#2,co)-y(b_b#2,co#2)=1e-4
c_e
l_e,,,
l-a-v
s_a_v 2 none
s_a_v 1 x(co) .35 .55,,
step,,
po
pl
```

Al-Co-Cr à 1400 °C

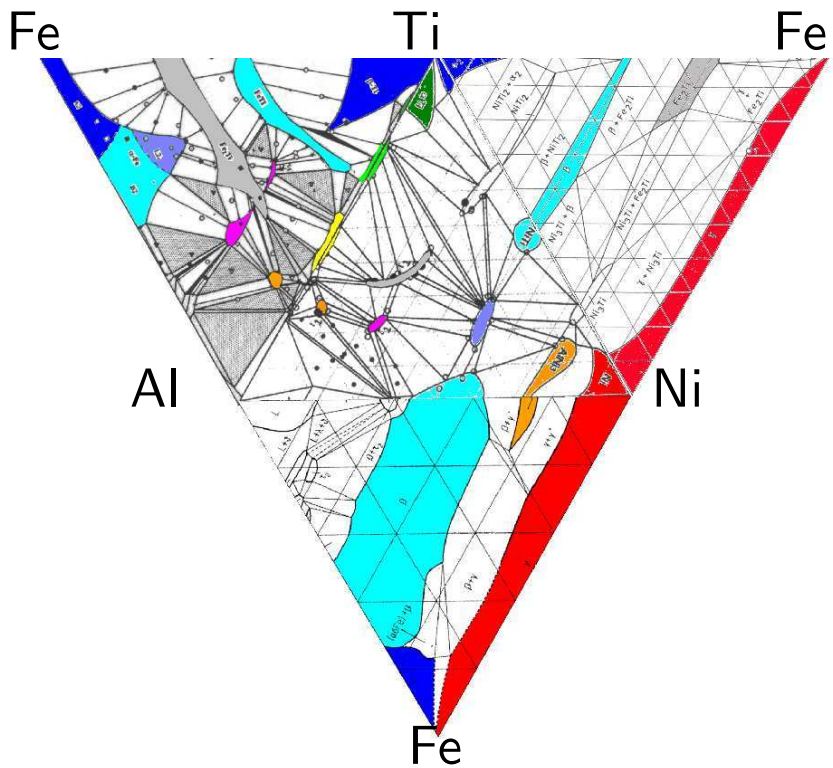
```
set_log alcocr1400
calcul metastable
go ter
```

```
b
l_c
s_c x(co)=.7 x(cr)=.1
```



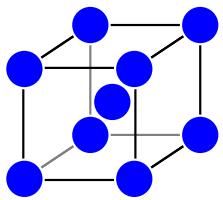

```
b
l_c
s_c x(co)=.5 x(cr)=.3
c_e
l_e,,,
ch_st p *=s
ch_st p bcc_b#2=e 1
adv glo n n
s_c x(cr)=none
s_c y(b_b#2,co)-y(b_b#2,co#2)=.1
c_e
l_e,,,
s_c y(b_b#2,co)-y(b_b#2,co#2)=1e-4
c_e
l_e,,,
l-a-v
s_a_v 2 none
s_a_v 1 x(co) .35 .55,,
step,,
po
pl
```

4 sous-réseaux

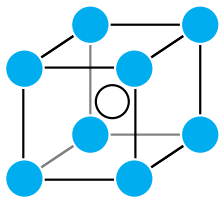


4 sous-réseaux

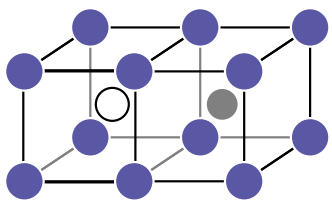
A2

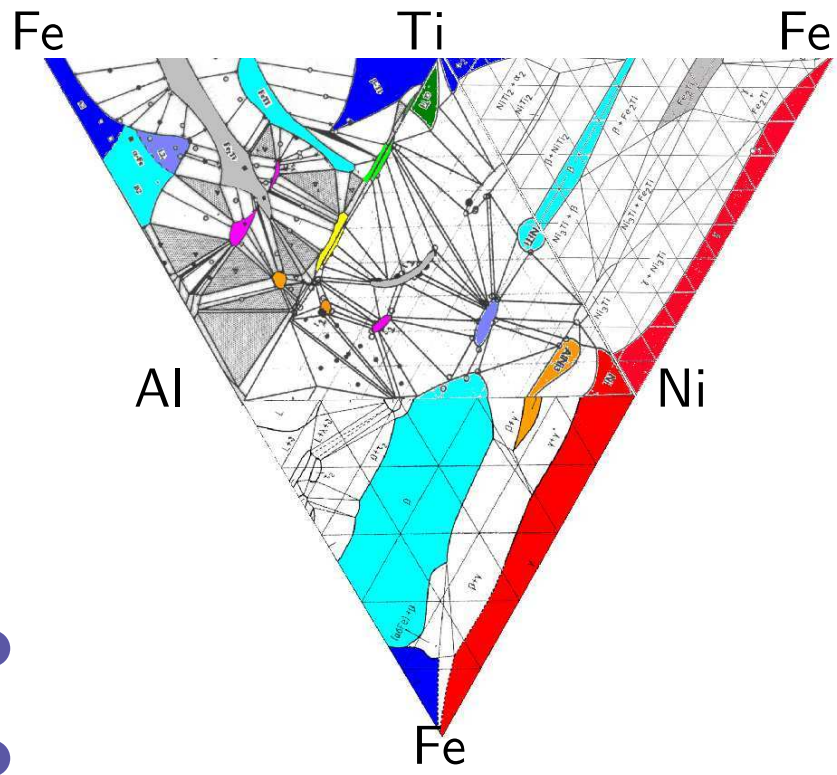


B2



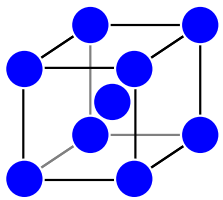
$L2_1$



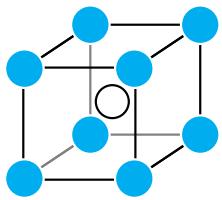


4 sous-réseaux

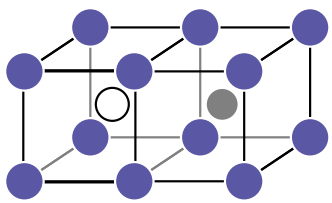
A2

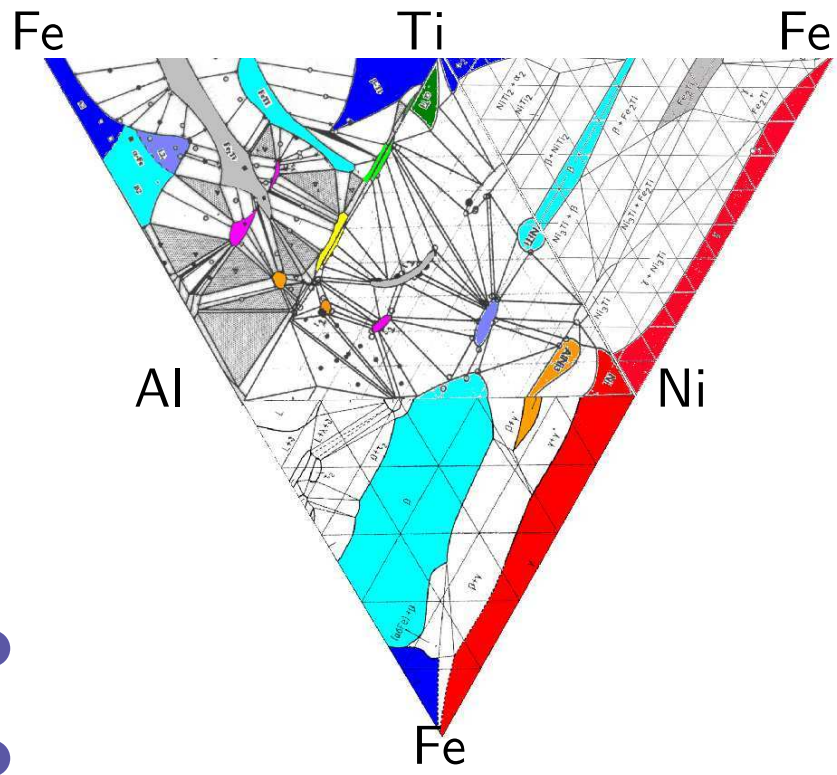


B2

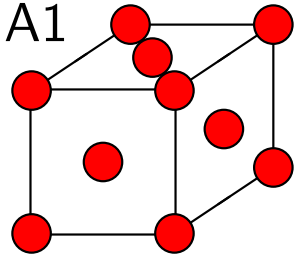


$L2_1$

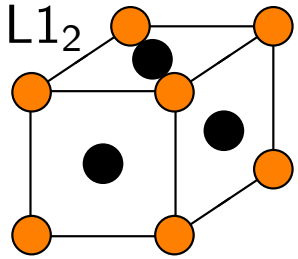




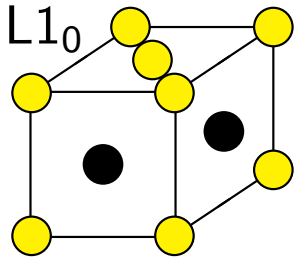
A1



$L1_2$

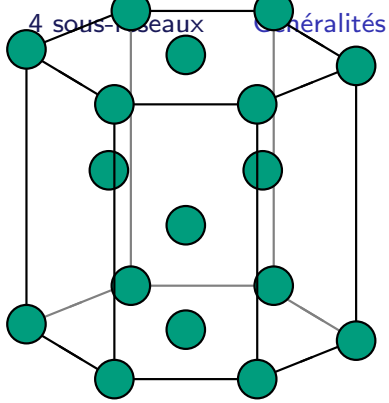


$L1_0$

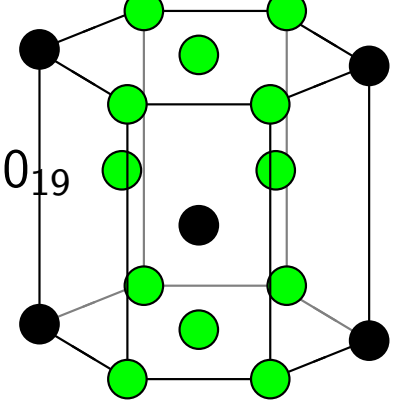


4 sous-réseaux

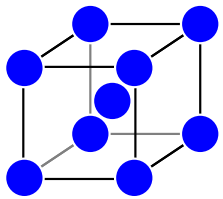
A3



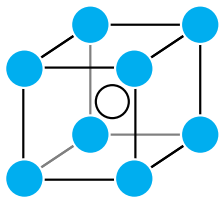
$D0_{19}$



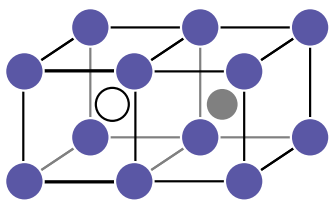
A2

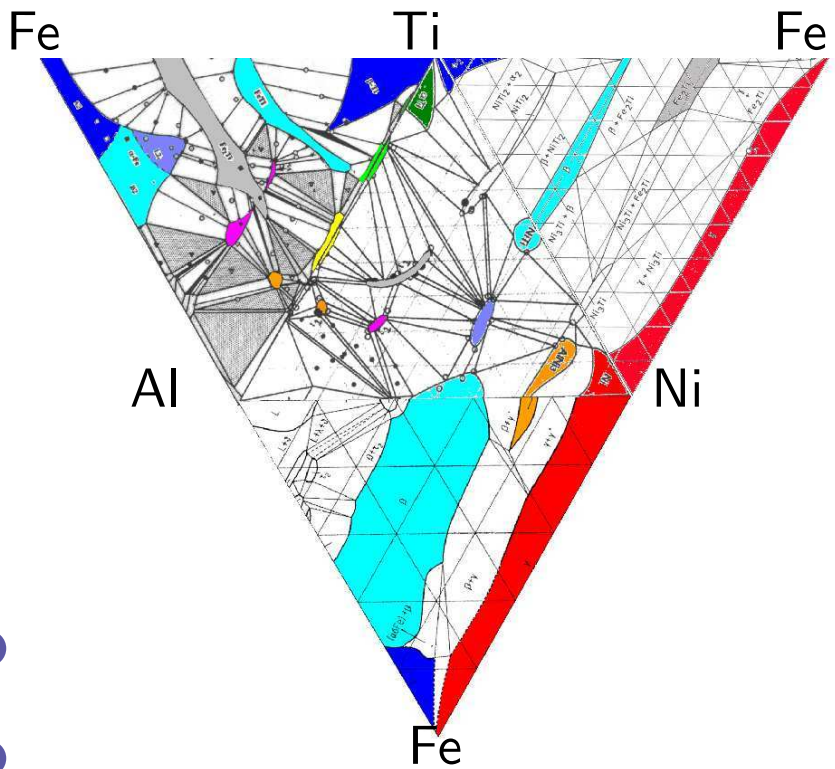


B2

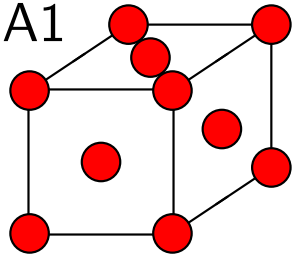


$L2_1$

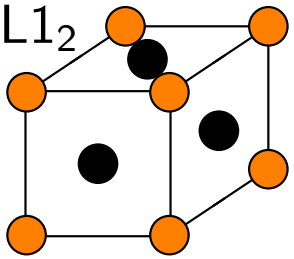




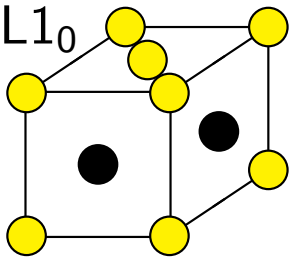
A1



$L1_2$



$L1_0$



4 sous-réseaux

Comme pour les modèles à deux sous-réseaux, l'enthalpie libre des différentes phases d'une même famille peut être décrite avec une seule expression, $G(y_i^s)$, fonction de l'occupation des différents sous-réseaux, y_i^s.

4 sous-réseaux

Comme pour les modèles à deux sous-réseaux, l'enthalpie libre des différentes phases d'une même famille peut être décrite avec une seule expression, $G(y_i^s)$, fonction de l'occupation des différents sous-réseaux, y_i^s.

(A,B)(A,B)(A,B)(A,B) fcc

$\rightsquigarrow$ $y_i^{(1)} = y_i^{(2)} = y_i^{(3)} = y_i^{(4)}$ $A1$

$\rightsquigarrow$ $y_i^{(1)} = y_i^{(2)} = y_i^{(3)} \neq y_i^{(4)}$ $L1_2$

$\rightsquigarrow$ $y_i^{(1)} = y_i^{(2)} \neq y_i^{(3)} = y_i^{(4)}$ $L1_0$

4 sous-réseaux

Comme pour les modèles à deux sous-réseaux, l'enthalpie libre des différentes phases d'une même famille peut être décrite avec une seule expression, $G(y_i^s)$, fonction de l'occupation des différents sous-réseaux, y_i^s.

(A,B)(A,B)(A,B)(A,B) bcc

$\rightsquigarrow$ $y_i^{(1)} = y_i^{(2)} = y_i^{(3)} = y_i^{(4)}$ $A2$

$\rightsquigarrow$ $y_i^{(1)} = y_i^{(2)} \neq y_i^{(3)} = y_i^{(4)}$ $B2$

$\rightsquigarrow$ $y_i^{(1)} = y_i^{(2)} \neq y_i^{(3)} = y_i^{(4)}$ $D0_3$ or $L2_1$

$\rightsquigarrow$ $y_i^{(1)} = y_i^{(3)} \neq y_i^{(2)} = y_i^{(4)}$ $B32$

4 sous-réseaux

Comme pour les modèles à deux sous-réseaux, l'enthalpie libre des différentes phases d'une même famille peut être décrite avec une seule expression, $G(y_i^s)$, fonction de l'occupation des différents sous-réseaux, y_i^s.

(A,B)(A,B)(A,B)(A,B) hcp

$\rightsquigarrow$ $y_i^{(1)} = y_i^{(2)} = y_i^{(3)} = y_i^{(4)}$ $A3$

$\rightsquigarrow$ $y_i^{(1)} = y_i^{(2)} = y_i^{(3)} \neq y_i^{(4)}$ $D0_{19}$

$\rightsquigarrow$ $y_i^{(1)} = y_i^{(2)} \neq y_i^{(3)} = y_i^{(4)}$ B_{19}

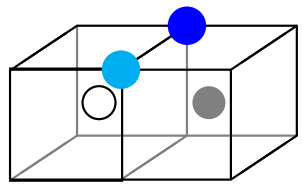
4 sous-réseaux

Comme pour les modèles à deux sous-réseaux, l'enthalpie libre des différentes phases d'une même famille peut être décrite avec une seule expression, $G(y_i^s)$, fonction de l'occupation des différents sous-réseaux, y_i^s.

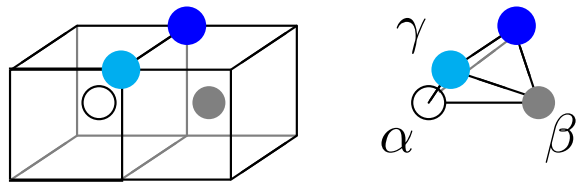
$$\begin{aligned} G(y_i^s) &= \sum_{ijkl} y_i^{(1)} y_j^{(2)} y_k^{(3)} y_l^{(4)} G_{i:j:k:l} \\ &\quad + \sum_s a^s \sum_i \ln y_i^s \\ &\quad + G^{xs} \end{aligned}$$

Des relations doivent être imposées entre les paramètres de l'enthalpie libre afin de permettre la stabilité du désordre. Celles-ci résultent simplement de la symétrie des réseaux crystallins considérés.

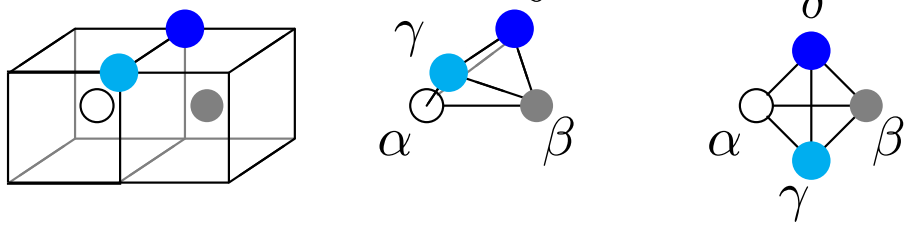
bcc 4 sous-réseaux



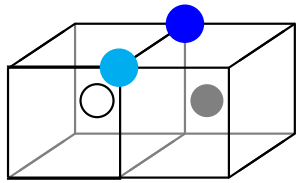
bcc 4 sous-réseaux

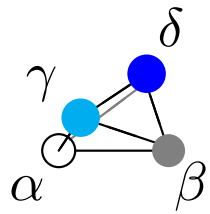


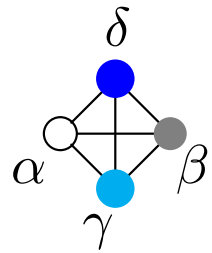
bcc 4 sous-réseaux



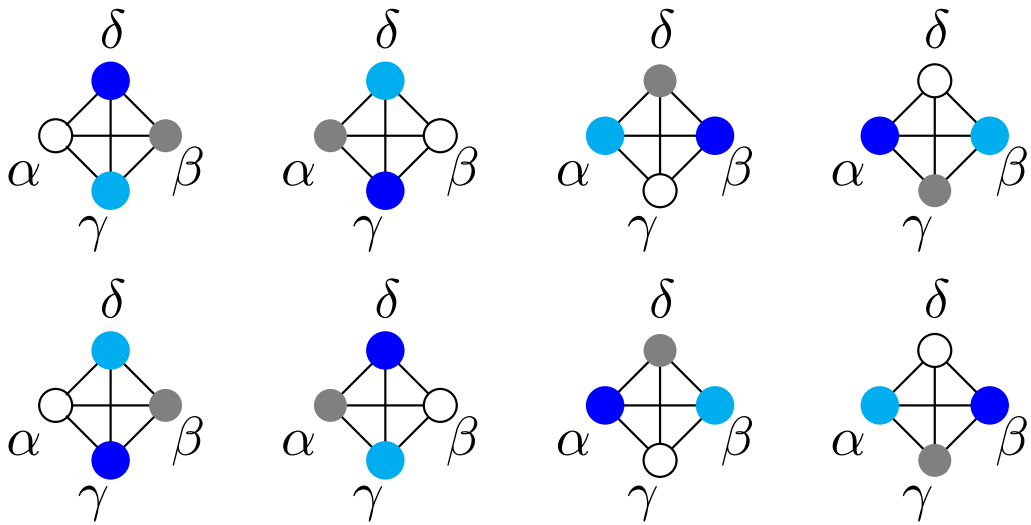
bcc 4 sous-réseaux



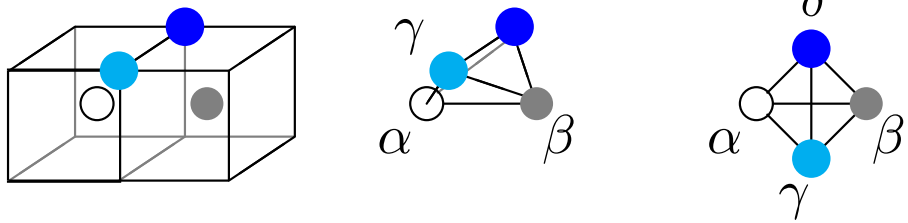




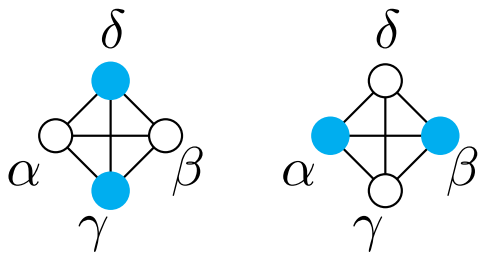
Du fait de la symétrie du réseau bcc,
ces configurations sont équivalentes.



bcc 4 sous-réseaux

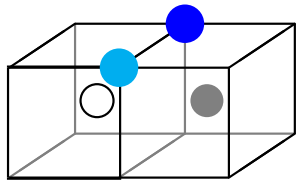


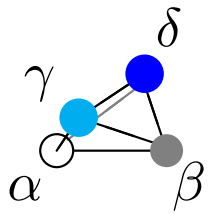
Du fait de la symétrie du réseau bcc,
ces configurations sont équivalentes.

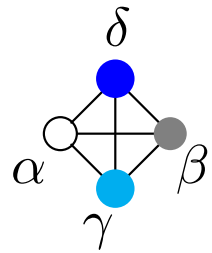


B2

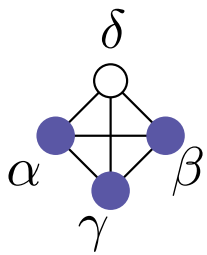
bcc 4 sous-réseaux

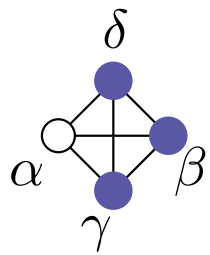


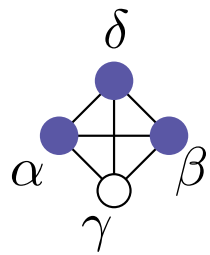


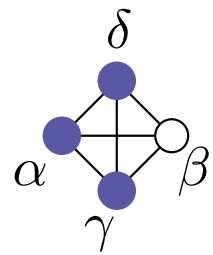


Du fait de la symétrie du réseau bcc,
ces configurations sont équivalentes.



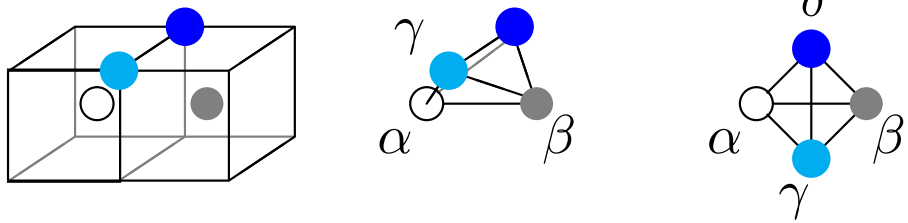




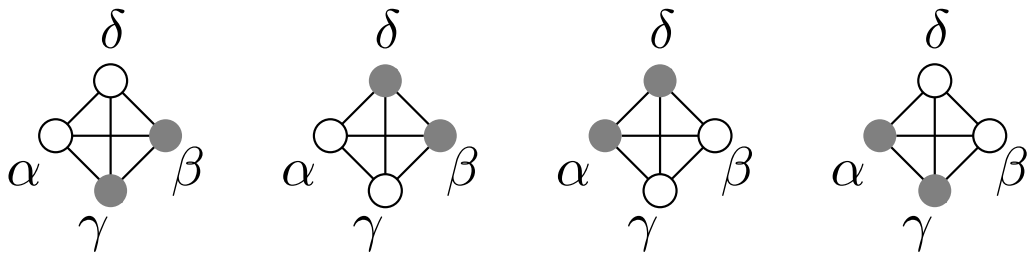


$D0_3$

bcc 4 sous-réseaux



Du fait de la symétrie du réseau bcc,
ces configurations sont équivalentes.

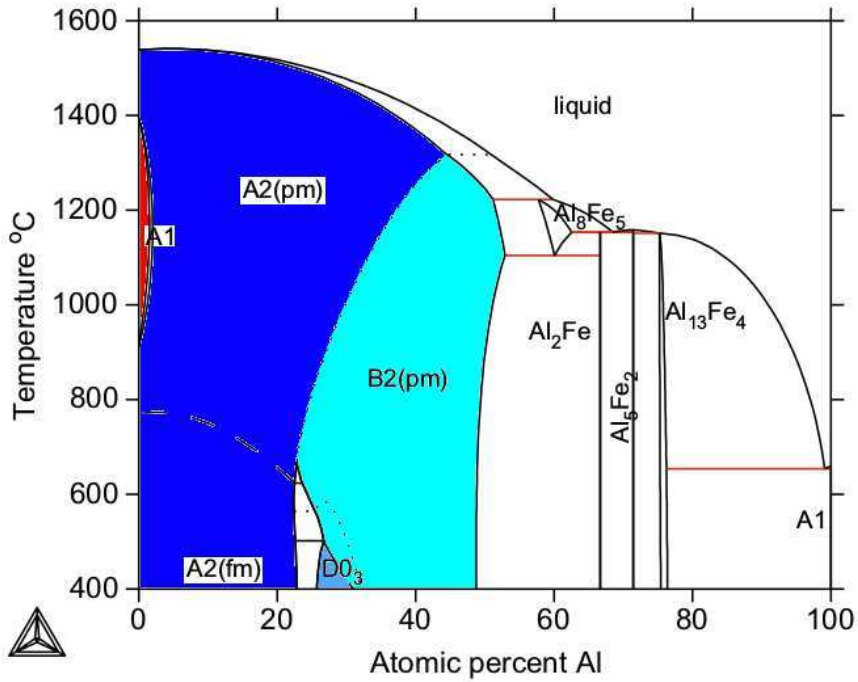


B32

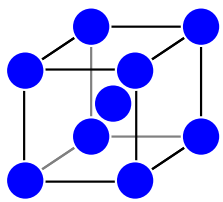
bcc 4 sous-réseaux

- L'assignation de la même enthalpie libre aux configurations équivalentes - enthalpies libres de formation des composés stœchiométriques et paramètres d'interaction - permet la stabilité de la phase désordonnée.
- Thermo-Calc présente une option - B - où l'équivalence des paramètres décrivant des configurations équivalentes basées sur le tétraèdre irrégulier constituant le réseau bcc est implicite.
- Cette option permet en outre une identification plus aisée de la nature des différentes phases.

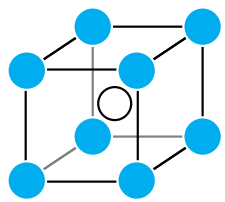
A2/B2/D0$_3$



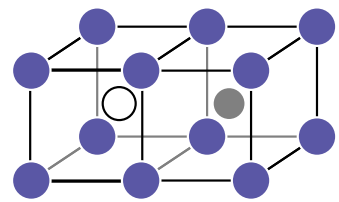
A2



B2

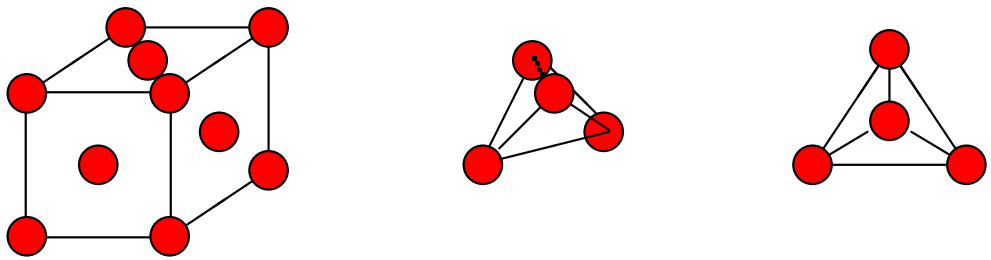


D0$_3$



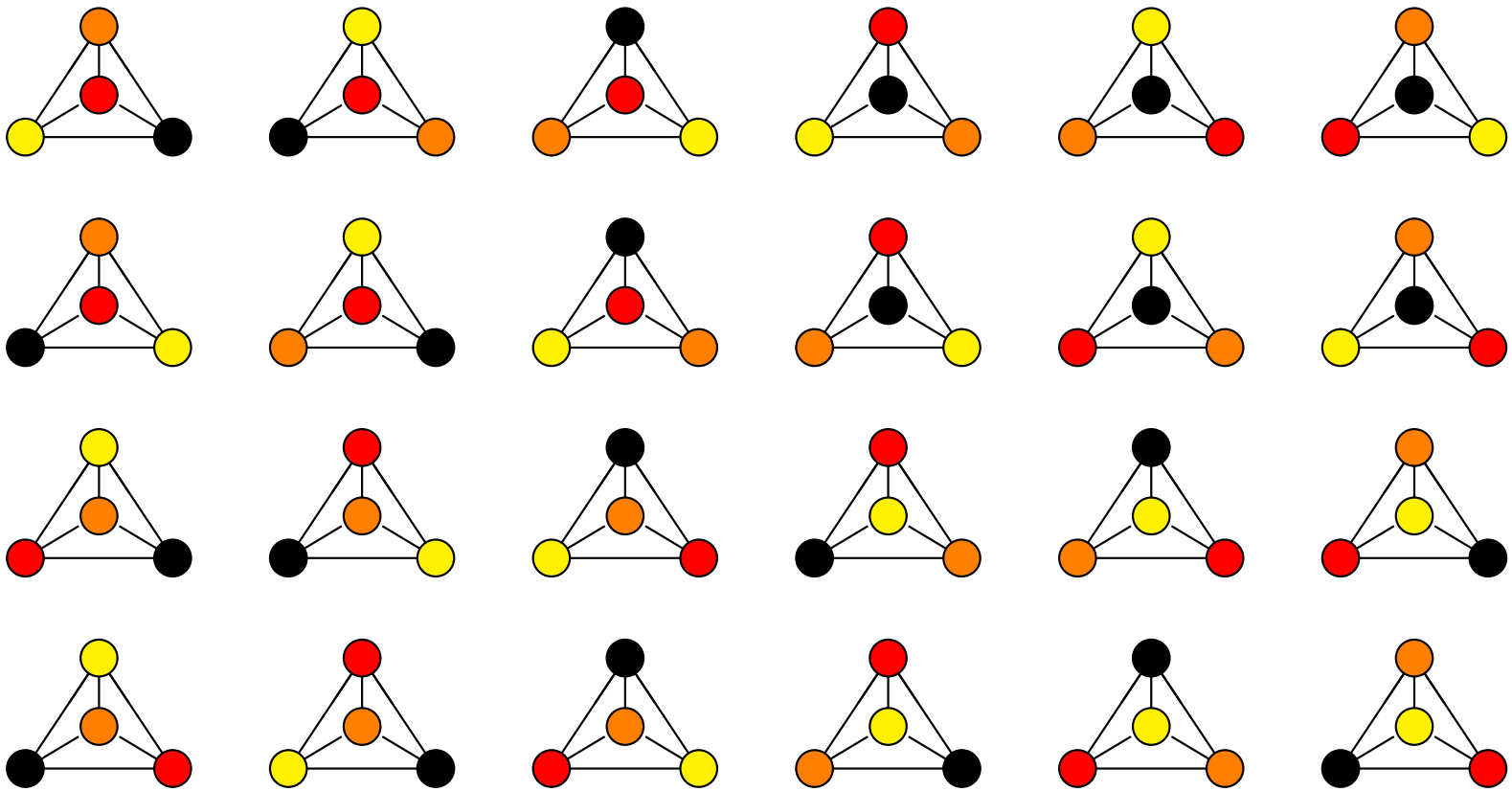
fcc 4 sous-réseaux

La description de la mise en ordre sur le réseau fcc avec 4 sous-réseaux est plus simple parce que basée sur des tétraèdres réguliers.



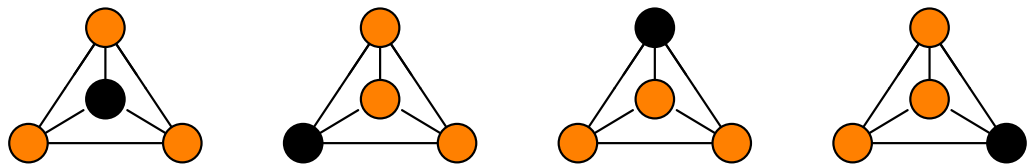
fcc 4 sous-réseaux

Du fait de la symétrie du réseau fcc,
ces configurations sont équivalentes.



fcc 4 sous-réseaux

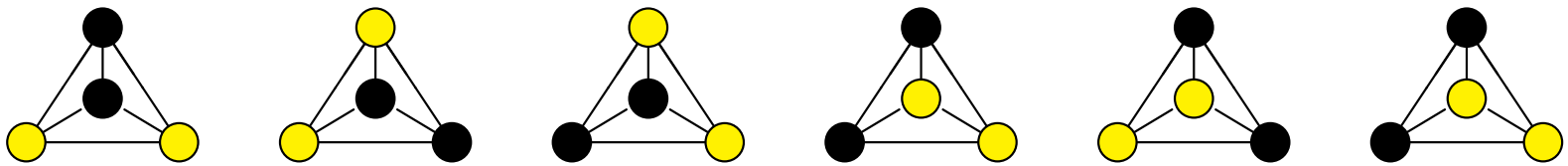
Du fait de la symétrie du réseau fcc,
ces configurations sont équivalentes.



$L1_2$

fcc 4 sous-réseaux

Du fait de la symétrie du réseau fcc,
ces configurations sont équivalentes.

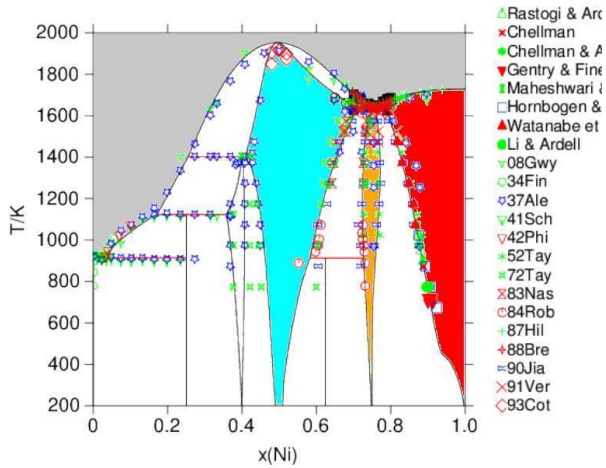


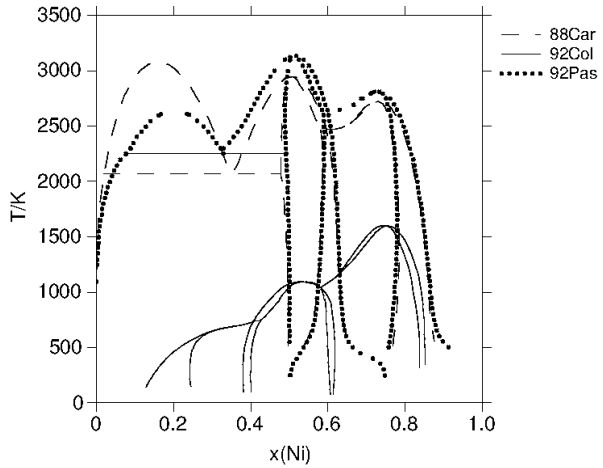
$L1_0$

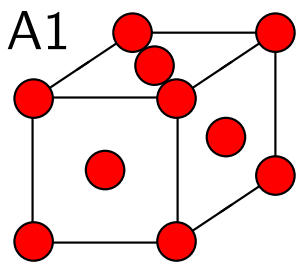
fcc 4 sous-réseaux

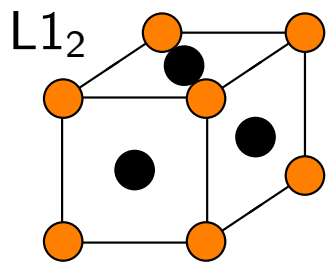
- Thermo-Calc présente une option - F - où l'équivalence des paramètres décrivant des configurations équivalentes basées sur le tétraèdre régulier constituant le réseau fcc est implicite.
- Cette option permet en outre une identification plus aisée de la nature des différentes phases.

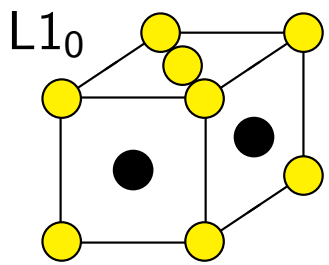
A1/L1$_2$

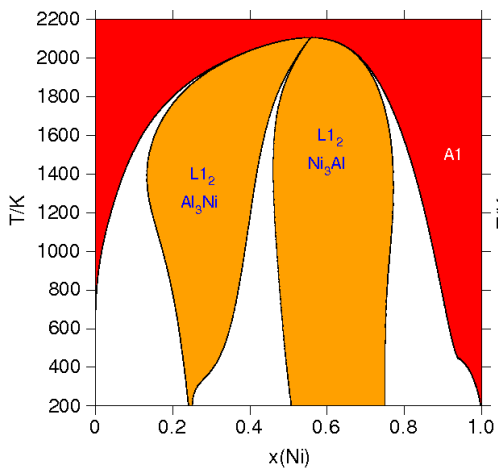

T/K
x(Ni)
Rastogi & Arc
Chellman
Chellman & A
Gentry & Fine
Maheshwari &
Hornbogen &
Watanabe et
Li & Ardell
08Gwy
34Fin
37Ale
41Sch
42Phi
52Tay
72Tay
83Nas
84Rob
87Hil
88Bre
90Jia
91Ver
93Cot

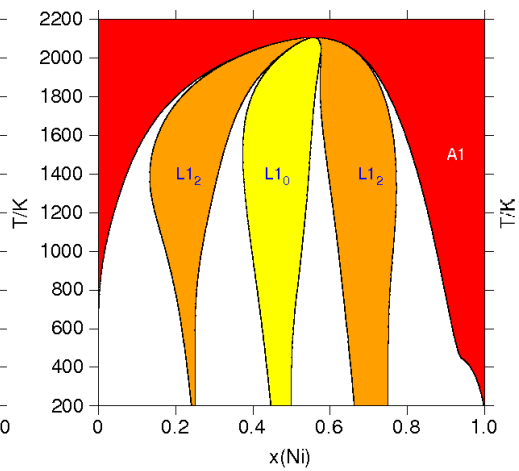

T/K
x(Ni)
88Car
92Col
92Pas

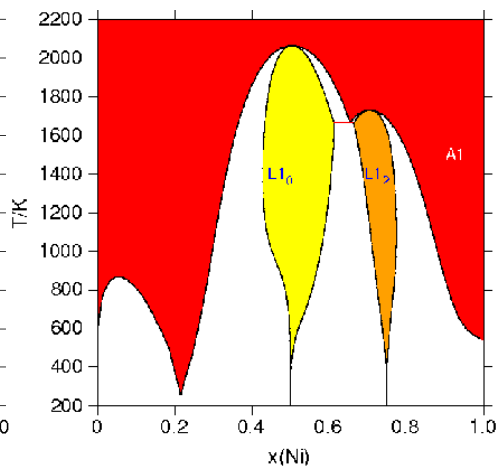

A1


L1$_2$


L1$_0$


T/K
x(Ni)
L1$_2$
Al$_3$Ni
L1$_2$
Ni$_3$Al
A1


T/K
x(Ni)
L1$_2$
L1$_0$
L1$_2$
A1


T/K
x(Ni)
L1$_0$
L1$_2$
A1

Al-Ni, Al-Fe

En utilisant les fichiers `AlFe_B.TDB` et `AlNi_F.TDB`, tracer

- pour Al-Fe, le diagramme stable, lignes de 2nd ordre comprises,
- pour Al-Ni, le diagramme métastable impliquant uniquement les phases de la famille fcc.