Modelling intermetallics Phases – II – Laves, μ and σ phases

Combining the Cluster Expansion and the Compound Energy formalisms

N. Dupin, S. Kussoffsky, S. G. Fries, W. A. Oates, and B. Sundman

Outline

Introduction

The Laves phase C15

$(A,B)_2\,(A,B) \rightarrow (A,B)_2\,(A,B)$

The μ phase

$(A,B)\,(A,B)_2\,(A)_6\,(B)_4 \rightarrow (A,B)\,(A,B)_2\,(A,B)_6\,(A,B)_4$

The σ phase

$(A)_8\,(B)_4\,(A,B)_{18} \rightarrow (A,B)_{10}\,(A,B)_4\,(A,B)_{16}$

Conclusion and perspectives

Introduction

- **Ordered phase, φ : (A, B, …)$_a$ (A, B, …)$_b$ …**

  - $G^{\varphi} = G(x) + G(y)$

with $G(x) = \sum_i x_i G_i^{\circ} + \sum_i \sum_j x_i x_j L_{i,j}^{x}$

$G(y) = RT \sum_s a^s \sum_i y_i^s \ln y_i^s + \sum_i \sum_j y_i^{'} y_j^{''} G_{i:j}^{y}$

$x_i = \sum_s a^s y_i^s$

The Laves Phase C15

Crystallography

Prototype	**Cu_2Mg**	
Space Group	$Fd\bar{3}m$	
Pearson Symbol	***cF24***	
Wyckhoff Position	***8(a)***	***16(d)***
Point Symmetry of Site	$\bar{4}3m$	$\bar{3}m$
Co-ordination Number	**16**	**12**
Site Occupation	**Mg**	**Cu**

The Laves Phase C15

Cu-Mg

- **Old CEF** (**Cu**,Mg)$_2$ (Cu,**Mg**)

$$G^{C15} = 3RT\sum_s a^s \sum_i x_i \ln x_i + \sum_i \sum_j y'_i y''_j G^{C15}_{i:j}$$
$$+ \sum_i \sum_j \sum_k y'_i y'_j y''_k L^{C15}_{i,j:k} + \sum_i \sum_j \sum_k y''_i y''_j y'_k L^{C15}_{k:i,j}$$

- $G^{C15}_{Cu:Cu}$ *and* $G^{C15}_{Mg:Mg}$ **fixed**
- $G^{C15}_{Cu:Mg}$, $L^{C15}_{Cu,Mg:Mg}$, *and* $L^{C15}_{Cu:Cu,Mg}$ **assessed**
- $G^{C15}_{Mg:Cu} = - G^{C15}_{Cu:Mg} + G^{C15}_{Cu:Cu} + G^{C15}_{Mg:Mg}$ **(WS)**

$$L^{C15}_{Cu,Mg:Cu} = L^{C15}_{Cu,Mg:Mg}, \quad L^{C15}_{Mg:Cu,Mg} = L^{C15}_{Cu:Cu,Mg}$$

The Laves Phase C15

- **New modelling** ($\mathbf{Cu}$,Mg)$_2$ (Cu,$\mathbf{Mg}$)

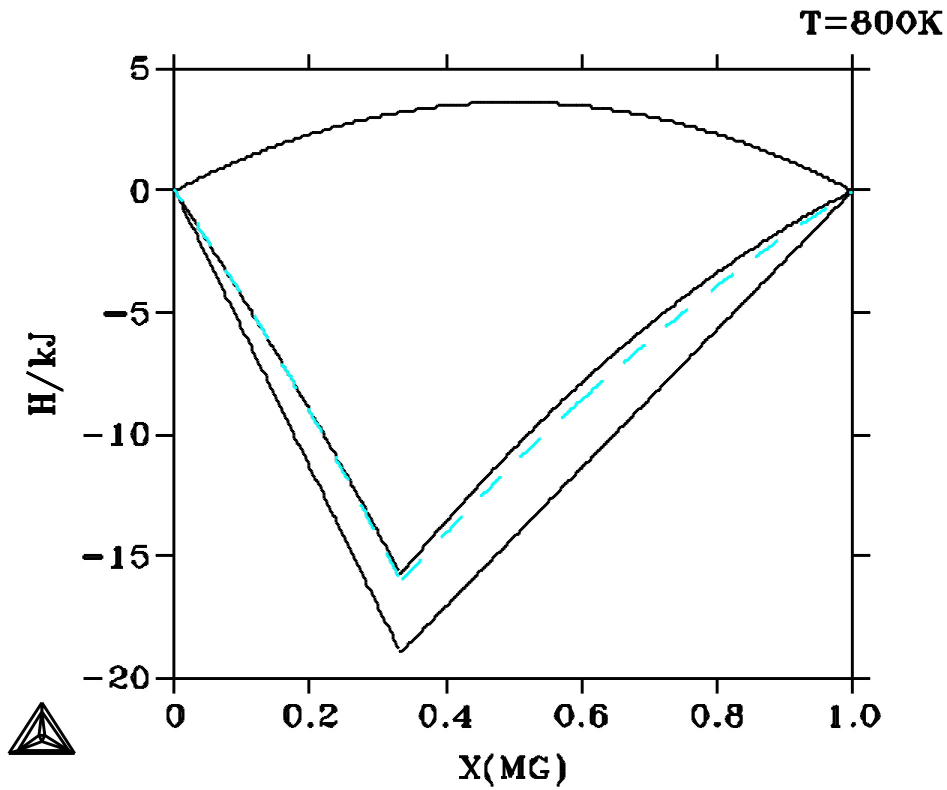
$$G^{C15} = \sum_i x_i G_i^{\circ} + \sum_i \sum_j x_i x_j L_{i,j}^{x}$$

$$+ RT \sum_s a^s \sum_i y_i^s \ln y_i^s + \sum_i \sum_j y'_i y''_j G_{i:j}^{y}$$

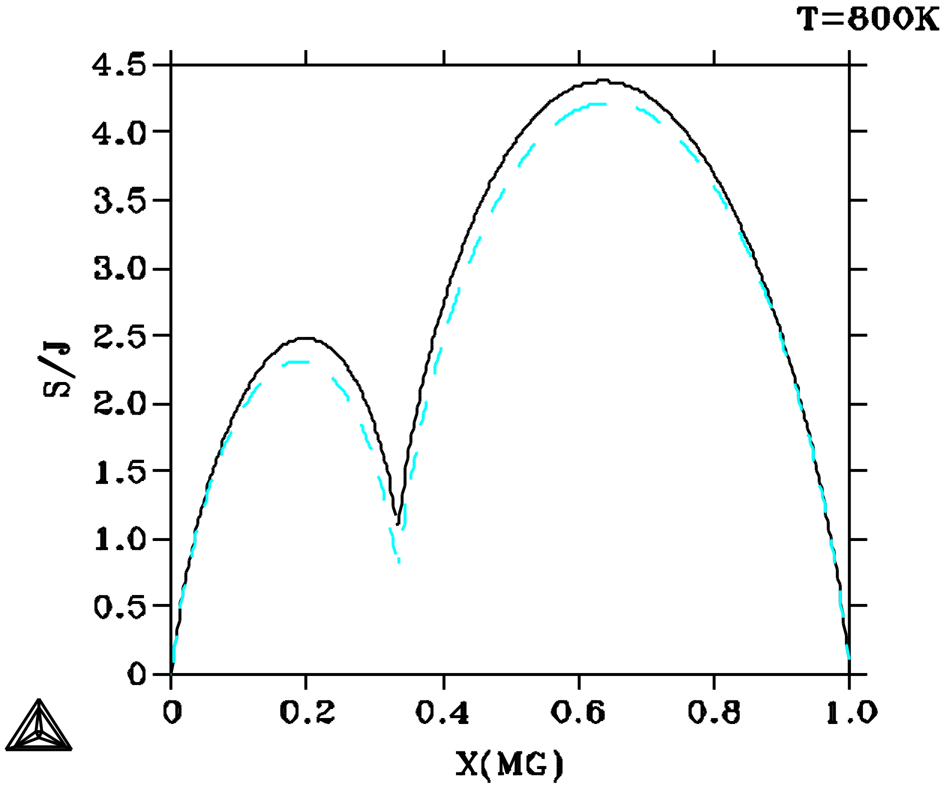
- $G_i^{\circ} = G_{i:i}^{C15} / 3$, $G_{i:i}^{y} = 0$ **fixed**
- $G_{Cu:Mg}^{y}$ *and* $L_{Cu,Mg}^{x}$ **assessed**
- $G_{Mg:Cu}^{y} = - G_{Cu:Mg}^{y}$
- **Using initial POP file + C_p**

The Laves Phase C15

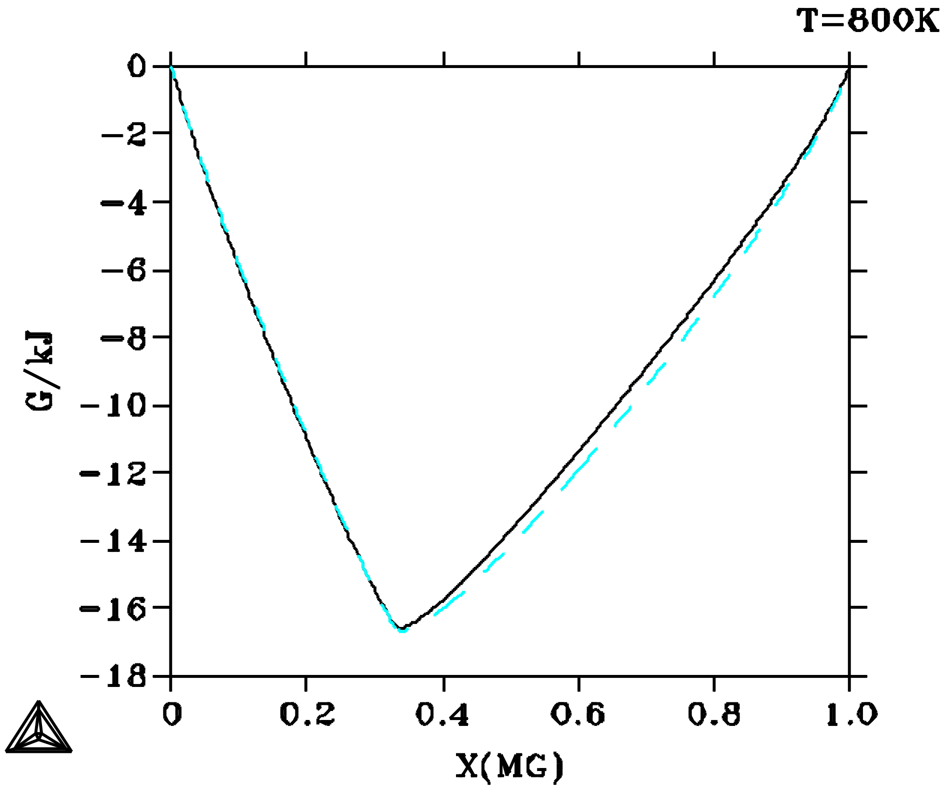
The Laves Phase C15



The Laves Phase C15



The Laves Phase C15



The Laves Phase C15

- **Al-Cu-Mg**

$(Al,Cu,Mg)_2\,(Al,Cu,Mg)$

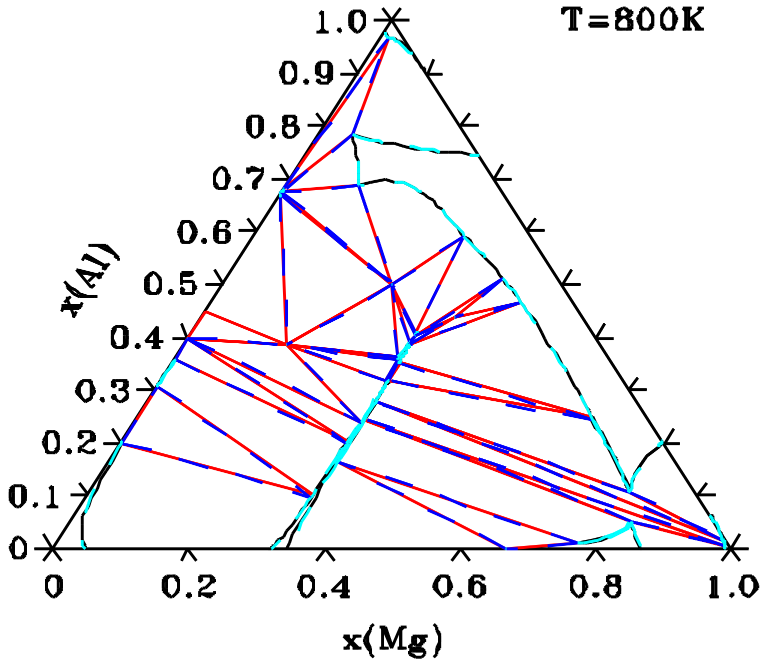
“old” description :

- **many parameters**
- **fixed / assessed parameters ?**

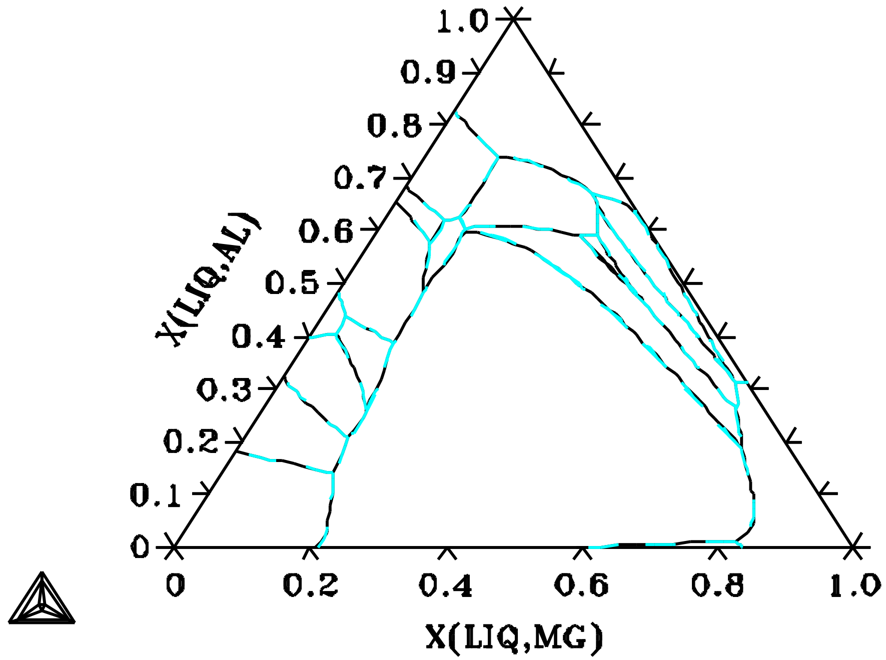
“new” description :

- **POP file had to be modified**
- **less parameters**

The Laves Phase C15



The Laves Phase C15



LAVES_C15
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
2 SUBLATTICES, SITES 1: 2
CONSTITUENTS: AL,CU,MG : AL,CU,MG

```
G(LAVES_C15,AL:AL;0)- 3 H298(FCC_A1,AL;0) = +15000+3*GHSERAL
G(LAVES_C15,CU:AL;0)- 2 H298(FCC_A1,AL;0)-H298(FCC_A1,CU;0) = +15000
    +2*GHSERAL+GHSERCU
G(LAVES_C15,MG:AL;0)- 2 H298(FCC_A1,AL;0)-H298(HCP_A3,MG;0) = +C15AL
    +2*GHSERAL+GHSERMG
G(LAVES_C15,AL:CU;0)-H298(FCC_A1,AL;0)- 2 H298(FCC_A1,CU;0) = +15000
    +2*GHSERCU+GHSERAL
G(LAVES_C15,CU:CU;0)- 3 H298(FCC_A1,CU;0) = +15000+3*GHSERCU
G(LAVES_C15,MG:CU;0)- 2 H298(FCC_A1,CU;0)-H298(HCP_A3,MG;0) =
    -54690.99+364.73085*T-69.276417*T*LN(T)-5.19246E-04*T**2
    +143502*T**(-1)-5.65953E-06*T**3
G(LAVES_C15,AL:MG;0)-H298(FCC_A1,AL;0)- 2 H298(HCP_A3,MG;0) =
    +104970.96-16.46448*T+2*GHSERMG+GHSERCU
G(LAVES_C15,CU:MG;0)-H298(FCC_A1,CU;0)- 2 H298(HCP_A3,MG;0) =
    +104970.96-16.46448*T+2*GHSERMG+GHSERCU
G(LAVES_C15,MG:MG;0)- 3 H298(HCP_A3,MG;0) = +15000+3*GHSERMG
```

L(LAVES_C15,AL,MG:AL;0) = +C15MGAL
L(LAVES_C15,AL:AL,CU;0) = +C15ALCU0+C15X
L(LAVES_C15,AL:AL,MG;0) = +C15ALMG0
L(LAVES_C15,CU,MG:AL;0) = +C15MGCU
L(LAVES_C15,CU:AL,CU;0) = +C15ALCU0+C15Y
L(LAVES_C15,CU:AL,MG;0) = +C15ALMG0
L(LAVES_C15,MG:AL,CU;0) = +C15ALCU0
L(LAVES_C15,MG:AL,MG;0) = +C15ALMG0
L(LAVES_C15,AL,MG:CU;0) = +C15MGAL
L(LAVES_C15,AL:CU,MG;0) = +C15CUMG0
L(LAVES_C15,CU,MG:CU;0) = +C15MGCU
L(LAVES_C15,CU:CU,MG;0) = +C15CUMG0
L(LAVES_C15,MG:CU,MG;0) = +C15CUMG0
L(LAVES_C15,AL,MG:MG;0) = +C15MGAL
L(LAVES_C15,CU,MG:MG;0) = +C15MGCU

```
DIS_C15
$ THIS PHASE IS THE DISORDERED PART OF LAVES_C15
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
   CONSTITUENTS: AL,CU,MG

     G(DIS_C15,AL;0)-H298(FCC_A1,AL;0) = +5000+GHSERAL
     G(DIS_C15,CU;0)-H298(FCC_A1,CU;0) = +5000+GHSERCU
     G(DIS_C15,MG;0)-H298(HCP_A3,MG;0) = +5000+GHSERMG
     L(DIS_C15,AL,CU;0) = +V1
     L(DIS_C15,AL,MG;0) = +V2
     L(DIS_C15,CU,MG;0) = 14530
```

LAVES_C15
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM DIS_C15
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: AL,CU,MG : AL,CU,MG

G(LAVES_C15,CU:AL;0)-H298(FCC,AL;0)- 2 H298(FCC,CU;0) = +V10
G(LAVES_C15,MG:AL;0)-H298(FCC,AL;0)- 2 H298(HCP,MG;0) = -V20-V22*T
G(LAVES_C15,AL:CU;0)- 2 H298(FCC,AL;0)-H298(FCC,CU;0) = +V10
G(LAVES_C15,MG:CU;0)-H298(FCC,CU;0)- 2 H298(HCP,MG;0) = -C15CUMG
G(LAVES_C15,AL:MG;0)- 2 H298(FCC,AL;0)-H298(HCP,MG;0) = +V20+V22*T
G(LAVES_C15,CU:MG;0)- 2 H298(FCC,CU;0)-H298(HCP,MG;0) = +C15CUMG

The μ Phase

Crystallography

Prototype	**Fe_7W_6**				
Space Group	$R\bar{3}m$				
Pearson Symbol	***hR 13***				
Wyckhoff Position	***1(a)***	***2(c)***	***2(c)***	***2(c)***	***6(h)***
Point Symmetry of Site	$\bar{3}m$	***3m***	***3m***	***3m***	***m***
Co-ordination Number	**12**	**15**	**16**	**14**	**12**
Site Occupation	**Fe**	**W**	**W**	**W**	**Fe**

The μ Phase

Co-Nb

- **Old CEF (Co,Nb) $(Co,Nb)_2$ $(Co)_6$ $(Nb)_4$**

$$G^{\mu} = 13\,RT \sum_s a^s \sum_i y_i^s \ln y_i^s + \sum_i \sum_j y'_i y''_j \, G^{\mu}_{i:j:Co:Nb}$$

- $G^{\mu}_{Co:Co:Co:Nb} = 7G^{fcc}_{Co} + 2G^{bcc}_{Co} + 4G^{bcc}_{Nb}$
- $G^{\mu}_{Co:Nb:Co:Nb} = 7G^{fcc}_{Co} + 6G^{bcc}_{Nb} + 13(V1 + V2T)$
- $G^{\mu}_{Nb:Nb:Co:Nb} = G^{fcc}_{Nb} + 6G^{fcc}_{Co} + 6G^{bcc}_{Nb} + 13(V1 + (V2 + V3)T)$
- $G^{\mu}_{Nb:Co:Co:Nb} = -\,G^{\mu}_{Co:Nb:Co:Nb} + G^{\mu}_{Co:Co:Co:Nb} + G^{\mu}_{Nb:Nb:Co:Nb}$
(WS)

The μ Phase

- **New modelling** (Co,Nb) $(Co,Nb)_2$ $(Co,Nb)_6$ $(Co,Nb)_4$

$$G^{\mu} = \sum_i x_i G_i^{\circ} + \sum_i \sum_j x_i x_j L_{i,j}^{x} + RT \sum_s a^s \sum_i y_i^s \ln y_i^s$$

$$+ \sum_i \sum_j \sum_k \sum_l y_i' y_j'' y_k''' y_l'''' G_{i:j:k:l}^{y}$$

- $G_i^{\circ} = \left(7G_i^{fcc} + 6G_i^{bcc}\right)/13$

- $G_{i:j:k:l}^{\mu} = 0$ except

  $G_{Co:Nb:Co:Nb}^{\mu} = V1 + V2T$

  $G_{Nb:Nb:Co:Nb}^{\mu} = V1 + (V2 + V3)T$

- V1, V2, V3 and $L_{Co,Nb}^{x}$ assessed using Kumar's POP file

The μ Phase

MU_PHASE
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
4 SUBLATTICES, SITES 1: 2: 6: 4
CONSTITUENTS: CO,NB : CO,NB : CO : NB

G(MU_PHASE,CO:CO:CO:NB;0) – 9 H298(HCP_A3,CO;0) – 4 H298(BCC_A2,NB;0) = + GB
G(MU_PHASE,NB:CO:CO:NB;0) – 8 H298(HCP_A3,CO;0) – 5 H298(BCC_A2,NB;0) = + GB + GC –GA
G(MU_PHASE,CO:NB:CO:NB;0) – 7 H298(HCP_A3,CO;0) – 6 H298(BCC_A2,NB;0) = + GA
G(MU_PHASE,NB:NB:CO:NB;0) – 6 H298(HCP_A3,CO;0) – 7 H298(BCC_A2,NB;0) = + GC

GA = +7*GCOFCC+6*GHSERNB+13*(–25810.7251+4.38850*T)
GB = +7*GCOFCC+2*GCOBCC+4*GHSERNB
GC = GNBFCC+6*GHSERNB+6*GCOFCC+13*(–25810.7251+(4.38850–0.52700) *T)

DIS_MU
$ THIS PHASE IS THE DISORDERED PART OF MU_PHASE
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: CO,NB

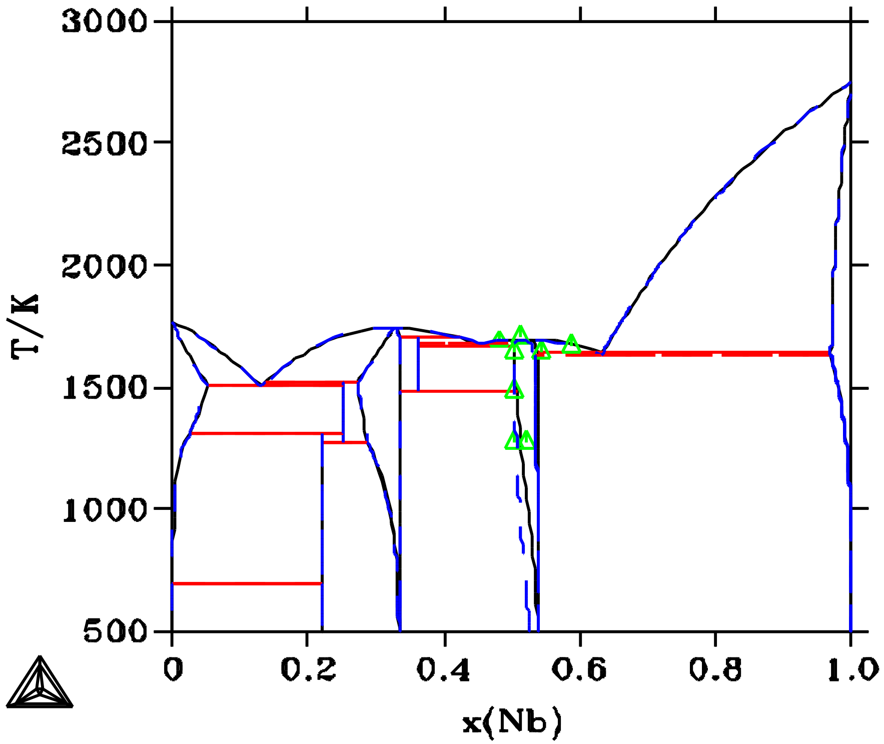
G(DIS_MU,CO;0)-H298(HCP_A3,CO;0) = +GMUA
G(DIS_MU,NB;0)-H298(BCC_A2,NB;0) = +GMUB
L(DIS_MU,CO,NB;0) = 125000

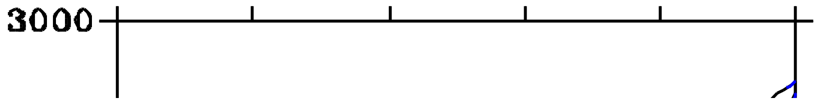
MU_PHASE
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM DIS_MU
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
4 SUBLATTICES, SITES 1: 2: 6: 4
CONSTITUENTS: CO,NB : CO,NB : CO,NB : CO,NB

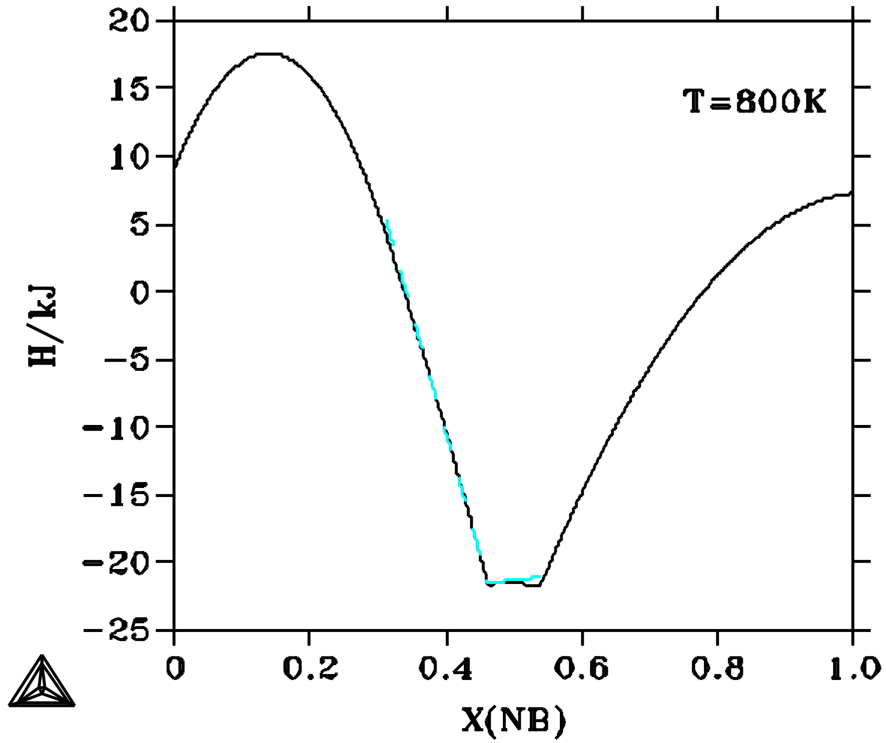
G(MU_PHASE,CO:NB:CO:NB;0)- 7 H298(HCP,CO;0)- 6 H298(BCC,NB;0) =
+13*GMUCO7NB
G(MU_PHASE,NB:NB:CO:NB;0)- 6 H298(HCP,CO;0)- 7 H298(BCC,NB;0) =
+13*(GMUCO7NB -0.079*T)

GMUCO7NB = -61000+3.97*T

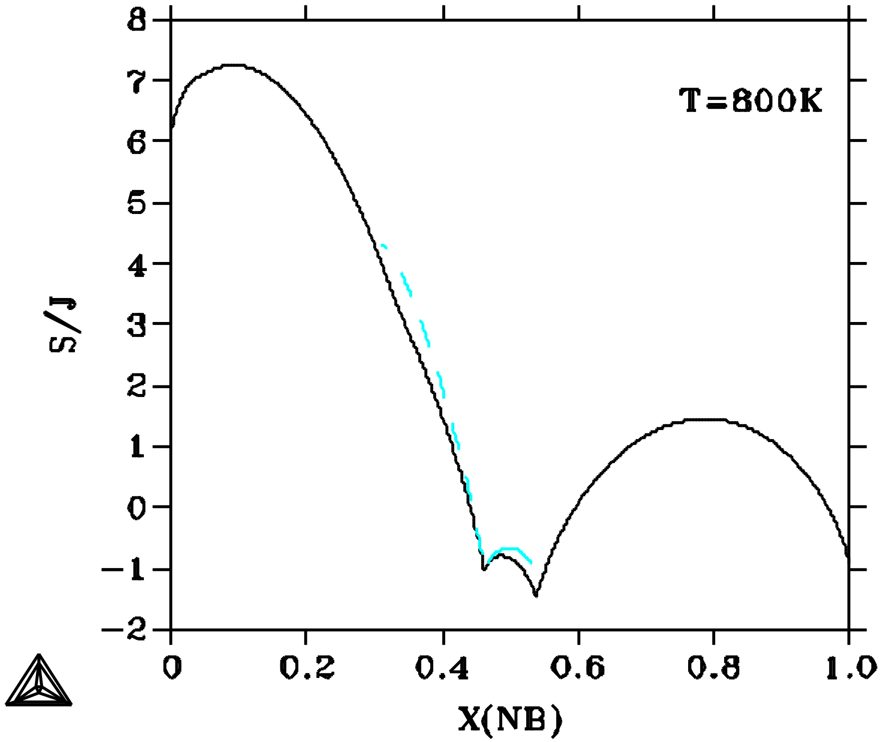
The μ Phase



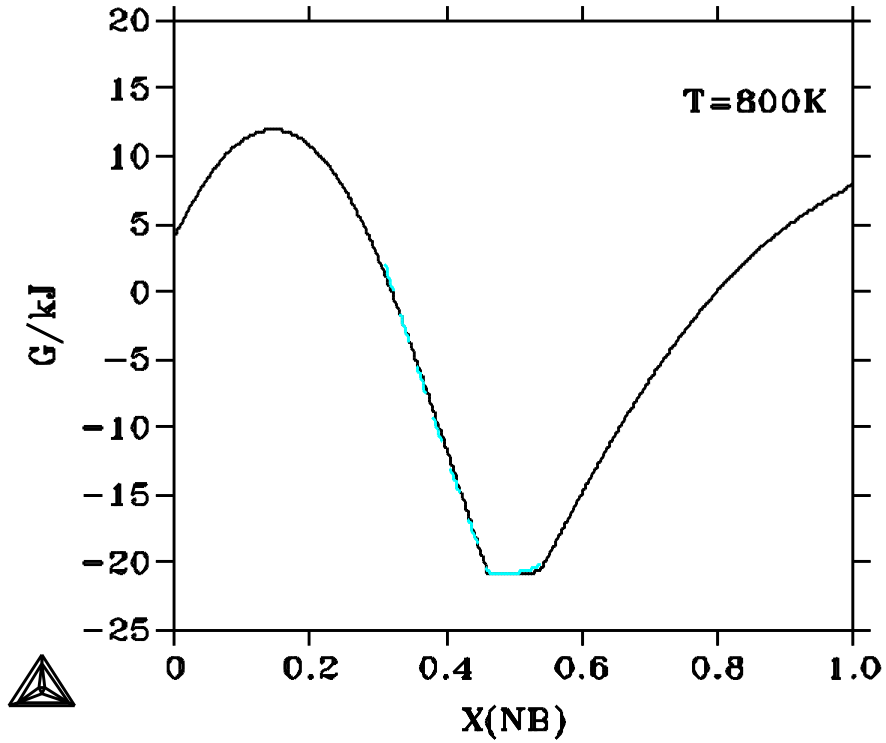

3000


T=800K
H/kJ
20
15
10
5
0
-5
-10
-15
-20
-25
0
0.2
0.4
0.6
0.8
1.0
X(NB)

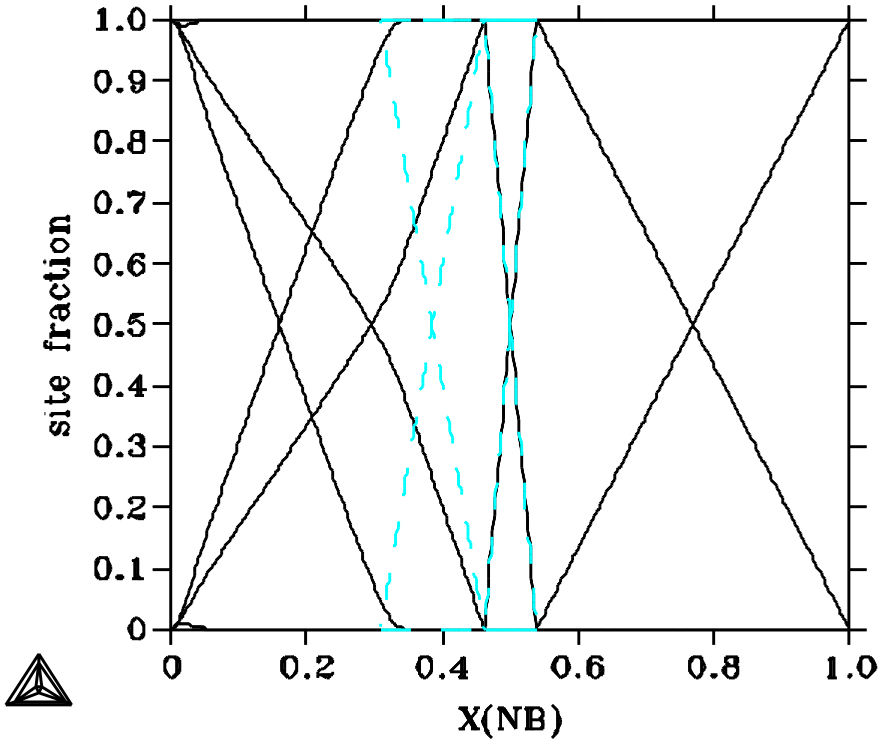
The μ Phase



The μ Phase



The μ Phase



The μ Phase

- New modelling (Co,Nb) $(Co,Nb)_2$ $(Co,Nb)_6$ $(Co,Nb)_4$

$$G^{\mu} = \sum_i x_i G_i^{\circ} + \sum_i \sum_j x_i x_j L_{i,j}^{x} + RT \sum_s a^s \sum_i y_i^s \ln y_i^s$$

$$+ \sum_i \sum_j \sum_k \sum_l y_i' y_j'' y_k''' y_l'''' G_{i:j:k:l}^{y}$$

- $G_i^{\circ} = (7G_i^{fcc} + 6G_i^{bcc})/13 + 50\,000$

- $G_{i:j:k:l}^{\mu} = 0$ except

  $G_{Co:Nb:Co:Nb}^{\mu} = V1 + V2T$

  $G_{Nb:Nb:Co:Nb}^{\mu} = V1 + (V2 + V3)T$

- V1, V2, V3 and $L_{Co,Nb}^{x}$ assessed using Kumar's POP file

DIS_MU

$ THIS PHASE IS THE DISORDERED PART OF MU_PHASE

EXCESS MODEL IS REDLICH-KISTER_MUGGIANU

CONSTITUENTS: CO,NB

G(DIS_MU,CO;0)-H298(HCP_A3,CO;0) = 50000 + GMUA

G(DIS_MU,NB;0)-H298(BCC_A2,NB;0) = 50000 + GMUB

L(DIS_MU,CO,NB;0) = –140000

MU_PHASE

$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM DIS_MU

EXCESS MODEL IS REDLICH-KISTER_MUGGIANU

4 SUBLATTICES, SITES 1: 2: 6: 4

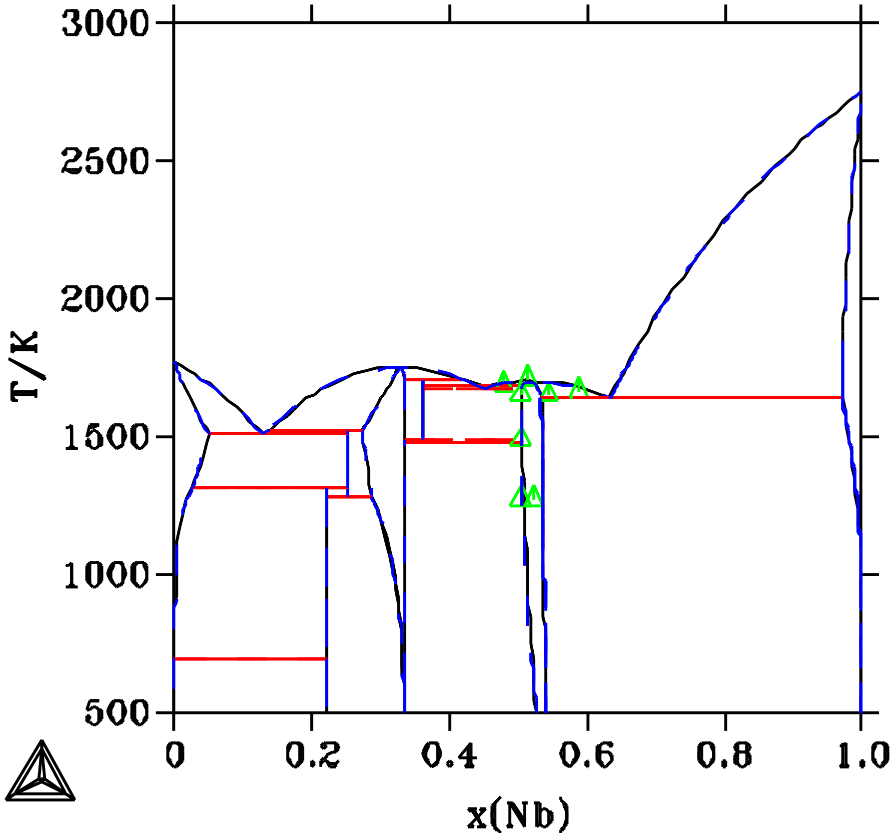
CONSTITUENTS: CO,NB : CO,NB : CO,NB : CO,NB

G(MU_PHASE,CO:NB:CO:NB;0)- 7 H298(HCP,CO;0)- 6 H298(BCC,NB;0) =
+13*GMUCO7NB

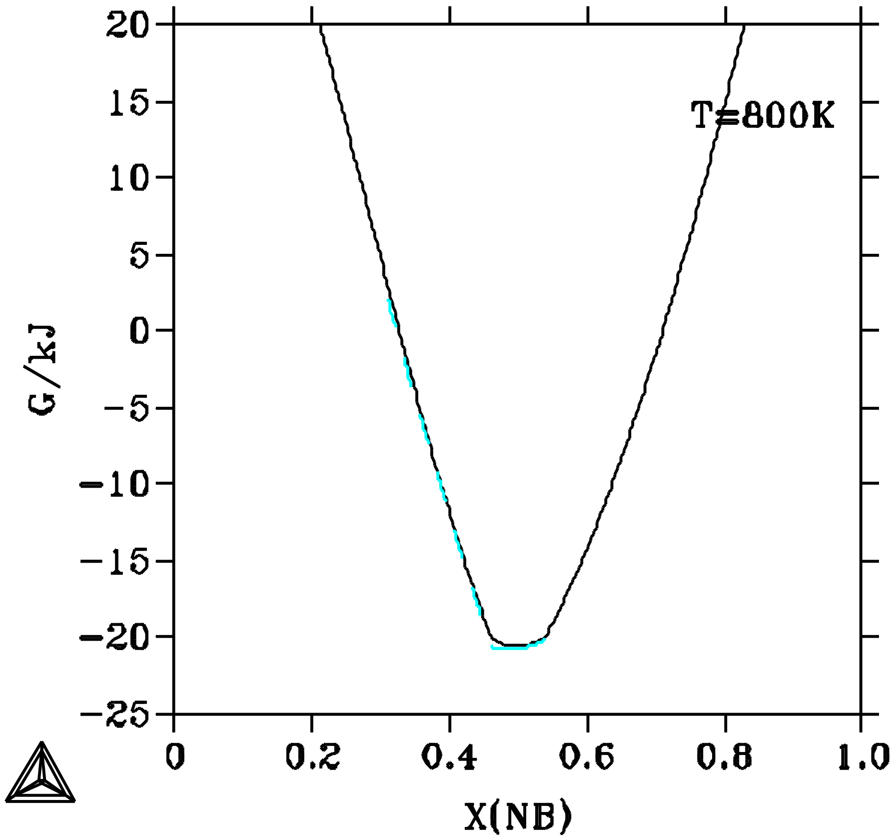
G(MU_PHASE,NB:NB:CO:NB;0)- 6 H298(HCP,CO;0)- 7 H298(BCC,NB;0) =
+13*(GMUCO7NB -0.22*T)

GMUCO7NB = –44200+3.68 *T

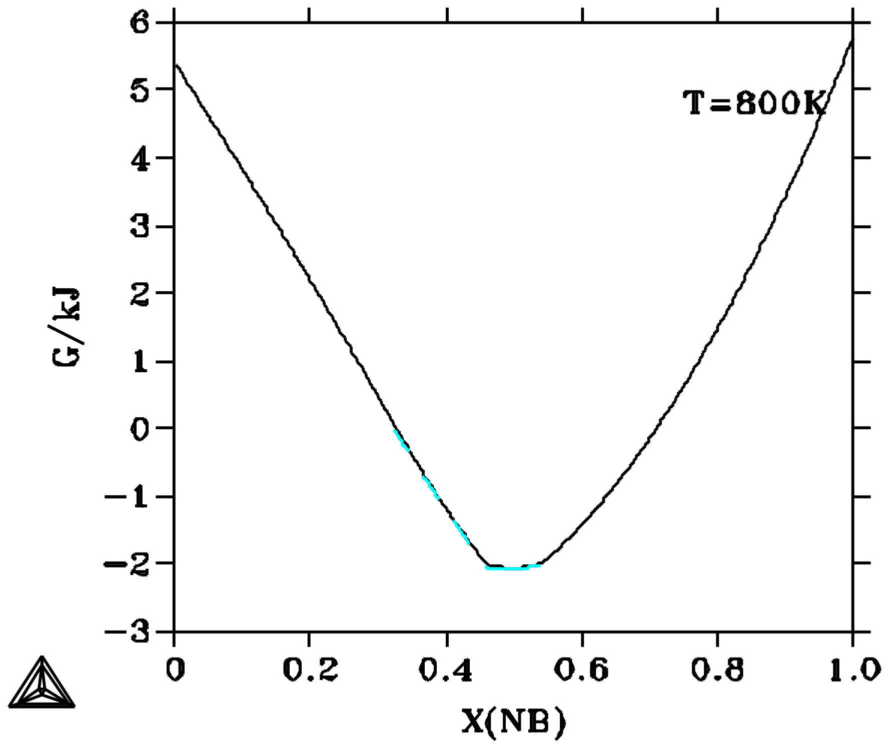
The μ Phase



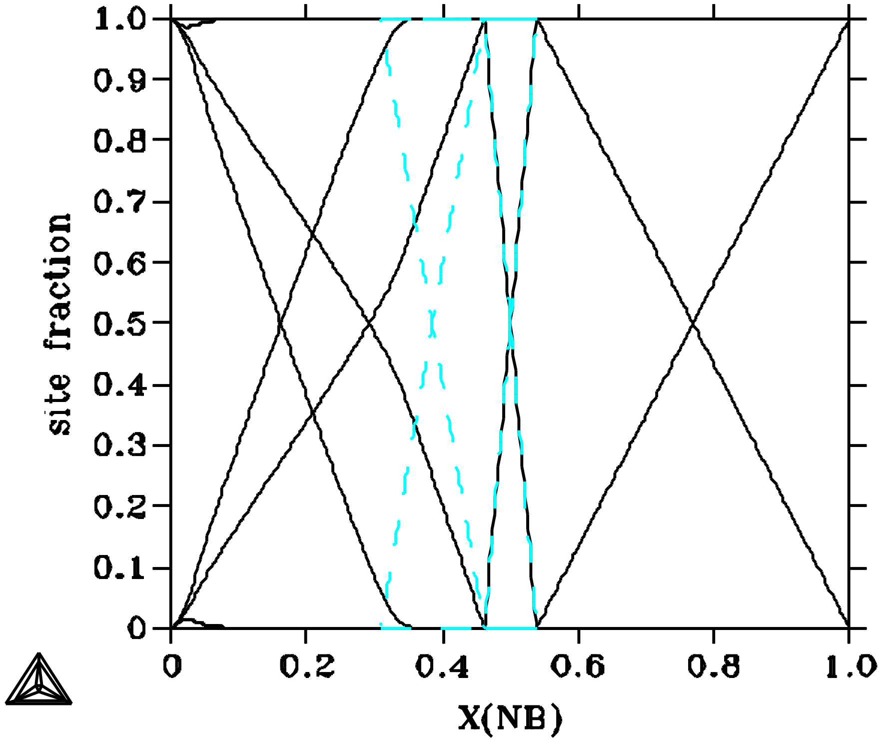
The μ Phase



The μ Phase



The μ Phase



MU_PHASE

$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM DIS_MU

EXCESS MODEL IS REDLICH-KISTER_MUGGIANU

4 SUBLATTICES, SITES 1: 2: 6: 4

CONSTITUENTS: CO,NB : CO,NB : CO,NB : CO,NB

G(MU_PHASE,CO:CO:CO:CO;0)- 13 H298(HCP,CO;0) = 0.0
G(MU_PHASE,NB:CO:CO:CO;0)- 12 H298(HCP,CO;0)-H298(BCC,NB;0) = 0.0
G(MU_PHASE,CO:NB:CO:CO;0)- 11 H298(HCP,CO;0)- 2 H298(BCC,NB;0) = 0.0
G(MU_PHASE,NB:NB:CO:CO;0)- 10 H298(HCP,CO;0)- 3 H298(BCC,NB;0) = 0.0
G(MU_PHASE,CO:CO:NB:CO;0)- 7 H298(HCP,CO;0)- 6 H298(BCC,NB;0) = 0.0
G(MU_PHASE,NB:CO:NB:CO;0)- 6 H298(HCP,CO;0)- 7 H298(BCC,NB;0) = 0.0
G(MU_PHASE,CO:NB:NB:CO;0)- 5 H298(HCP,CO;0)- 8 H298(BCC,NB;0) = 0.0
G(MU_PHASE,NB:NB:NB:CO;0)- 4 H298(HCP,CO;0)- 9 H298(BCC,NB;0) = 0.0
G(MU_PHASE,CO:CO:CO:NB;0)- 9 H298(HCP,CO;0)- 4 H298(BCC,NB;0) = 0.0
G(MU_PHASE,NB:CO:CO:NB;0)- 8 H298(HCP,CO;0)- 5 H298(BCC,NB;0) = 0.0
G(MU_PHASE,CO:NB:CO:NB;0)- 7 H298(HCP,CO;0)- 6 H298(BCC,NB;0) =
+13*GMUCO7NB
G(MU_PHASE,NB:NB:CO:NB;0)- 6 H298(HCP,CO;0)- 7 H298(BCC,NB;0) =
+13*GMUCO6NB
G(MU_PHASE,CO:CO:NB:NB;0)- 3 H298(HCP,CO;0)- 10 H298(BCC_A2,NB;0) = 0.0
G(MU_PHASE,NB:CO:NB:NB;0)- 2 H298(HCP,CO;0)- 11 H298(BCC_A2,NB;0) = 0.0
G(MU_PHASE,NB:CO:NB:NB;0)- 2 H298(HCP,CO;0)- 11 H298(BCC,NB;0) = 0.0
G(MU_PHASE,CO:NB:NB:NB;0)-H298(HCP,CO;0)- 12 H298(BCC,NB;0) = 0.0
G(MU_PHASE,NB:NB:NB:NB;0)- 13 H298(BCC,NB;0) = 0.0

The σ Phase

Crystallography

Prototype	**CrFe**					
Space Group	$P\ 4_2/mnm$					
Pearson Symbol	***tP30***					
Wyckhoff Position		***2(a)***	***4(f)***	***8(i)***	***8(i)***	***8(j)***
Point Symmetry of Site		***mmm***	***mm***	***m***	***m***	***m***
Co-ordination Number		**12**	**15**	**14**	**12**	**14**
Site Occupation Fe		**88**	**25**	**38**	**84**	**34**

The σ Phase

Cr-Fe

- **Old CEF** $(Fe)_8\,(Cr)_4\,(Fe,Cr)_{18}$

$$G^{\sigma} = 18\,RT \sum_i y_i''' \ln y_i''' + \sum_i y_i''' G^{\sigma}_{Fe:Cr:i}$$

  - $G^{\sigma}_{Fe:Cr:Cr} = 8G^{fcc}_{Fe} + 22G^{bcc}_{Cr} + A + BT$
  - $G^{\sigma}_{Fe:Cr:Fe} = 8G^{fcc}_{Fe} + 4G^{bcc}_{Cr} + 18G^{bcc}_{Fe} + A' + BT$

The σ Phase

- **New modelling $(Fe,Cr)_{10}\ (Fe,Cr)_4\ (Fe,Cr)_{16}$**

$$G^{\sigma} = \sum_i x_i G_i^{\circ} + \sum_i \sum_j x_i x_j L_{i,j}^{x} + RT \sum_s a^s \sum_i y_i^s \ln y_i^s$$

$$+ \sum_i \sum_j \sum_k y_i' y_j'' y_k''' G_{i:j:k}^{y}$$

- $G_i^{\circ} = \left(10 G_i^{fcc} + 20 G_i^{bcc}\right) / 30$

- $G_{i:j:k}^{y} = 0$ **except**

  $G_{Fe:Cr:Cr}^{y} = A + B\,T$

  $G_{Fe:Cr:Fe}^{y} = A' + B'T$

- **A, A', B, B' and $L_{Cr,Fe}^{x}$ assessed using *calculated* POP file**

The σ Phase

- **New modelling $(Fe,Cr)_{10}$ $(Fe,Cr)_4$ $(Fe,Cr)_{16}$**

$$G^{\sigma} = \sum_i x_i G_i^{\circ} + \sum_i \sum_j x_i x_j L_{i,j}^{x} + RT \sum_s a^s \sum_i y_i^s \ln y_i^s$$

$$+ \sum_i \sum_j \sum_k y_i' y_j'' y_k''' G_{i:j:k}^{y}$$

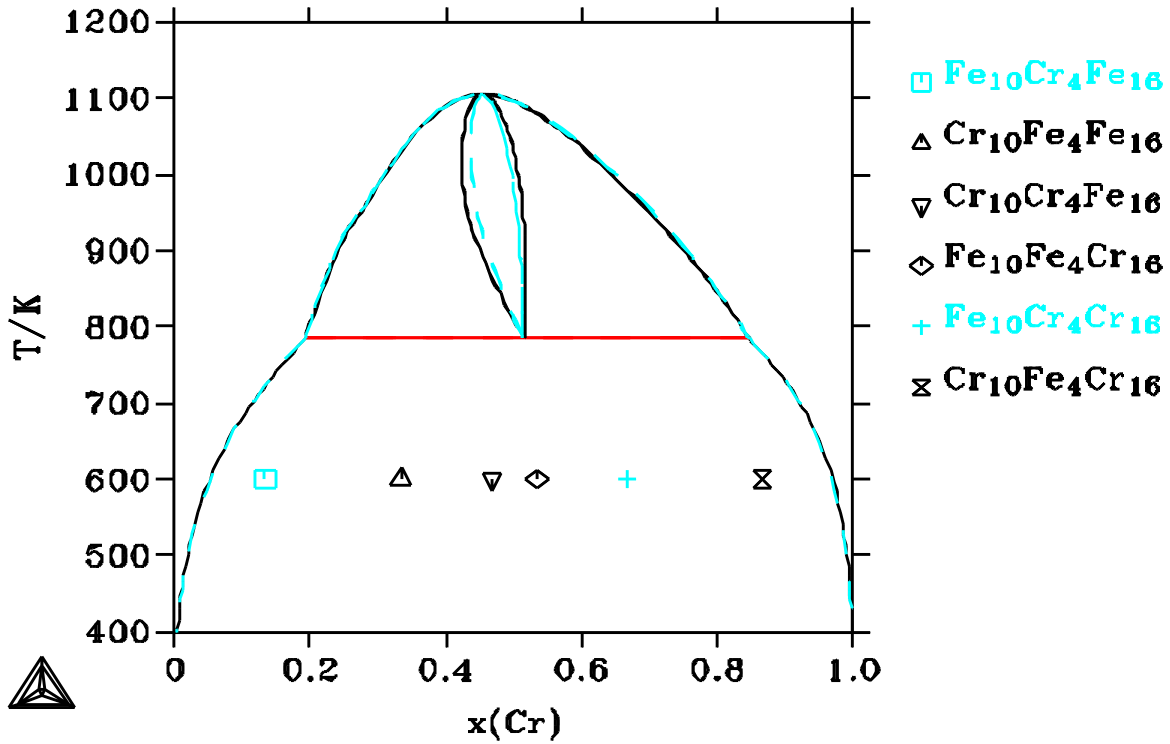
- $G_i^{\circ} = (10G_i^{fcc} + 20G_i^{bcc})/30 + 2000$

- $G_{i:j:k}^{y} = 0$ **except**

  $G_{Fe:Cr:Cr}^{y}$ ***and*** $G_{Fe:Cr:Fe}^{y}$

- $G_{Fe:Cr:Cr}^{y}$, $G_{Fe:Cr:Fe}^{y}$ **and** $L_{Cr,Fe}^{x}$ **assessed using *calculated* POP file**

The σ Phase



1200
1100
1000
900
800
700
600
500
400
T/K
0
0.2
0.4
0.6
0.8
1.0
x(Cr)
Fe10Cr4Fe16
Cr10Fe4Fe16
Cr10Cr4Fe16
Fe10Fe4Cr16
Fe10Cr4Cr16
Cr10Fe4Cr16

The σ Phase

- **New modelling $(Fe,Cr)_{10}$ $(Fe,Cr)_{4}$ $(Fe,Cr)_{16}$**

$$G^{\sigma} = \sum_i x_i G_i^{\circ} + \sum_i \sum_j x_i x_j L_{i,j}^{x} + RT \sum_s a^s \sum_i y_i^s \ln y_i^s$$

$$+ \sum_i \sum_j \sum_k y_i' y_j'' y_k''' G_{i:j:k}^{y}$$

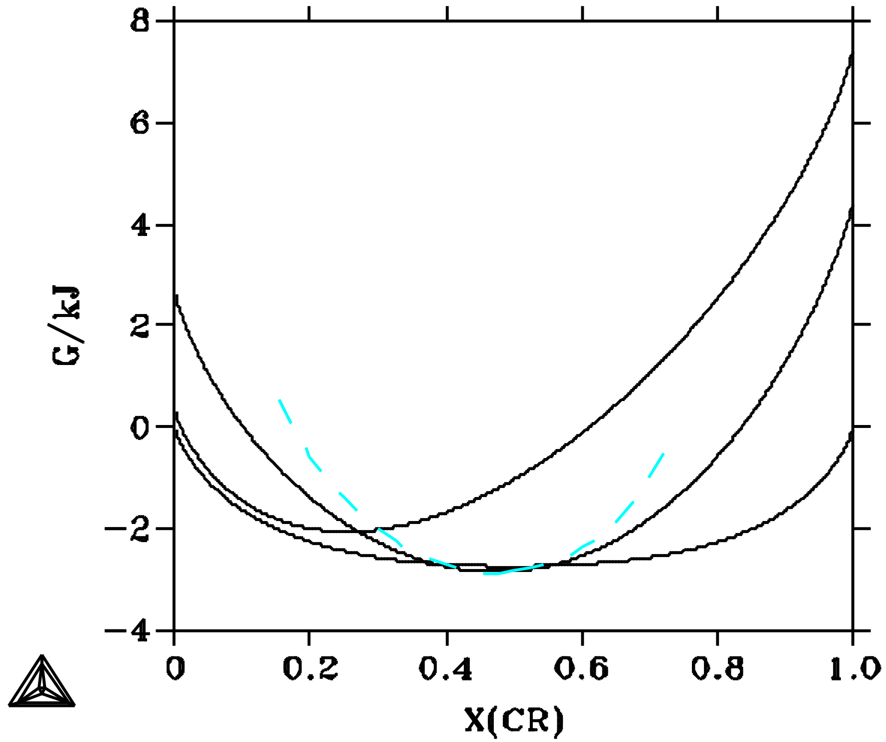
- $L_{Cr,Fe}^{x} = 0$

- $G_i^{\circ} = (10 G_i^{fcc} + 20 G_i^{bcc}) / 30 + V1$

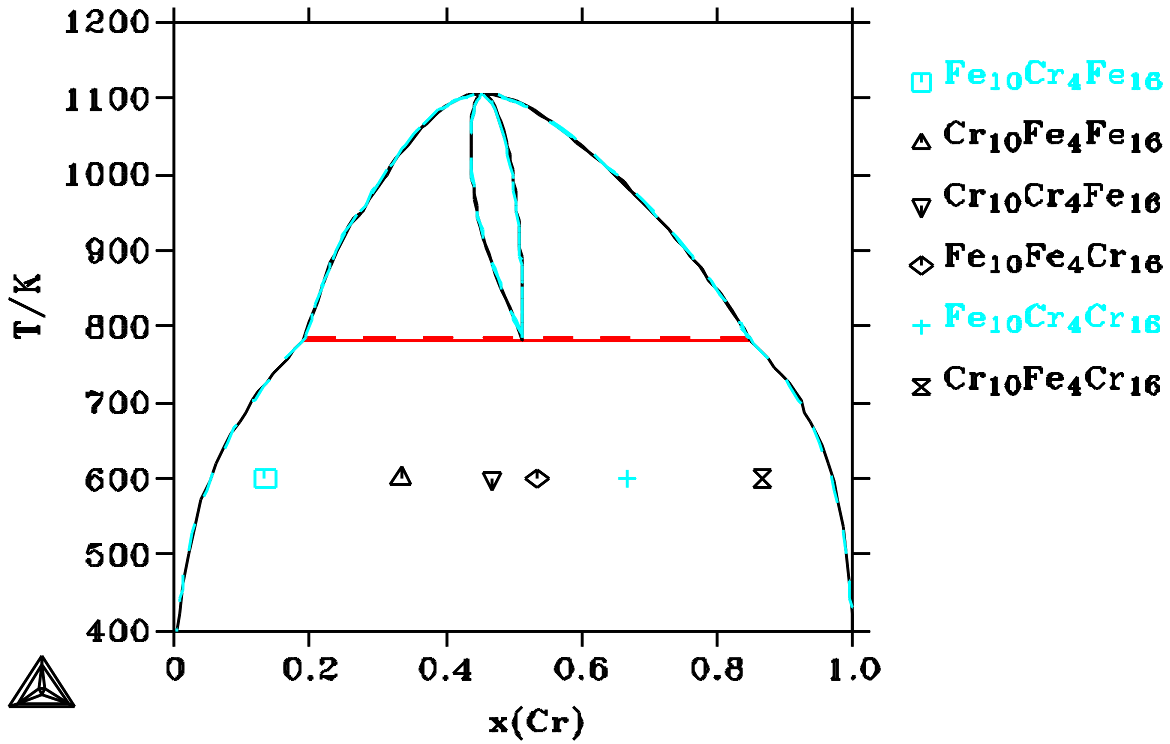
- $G_{i:j:k}^{y} = 0$ except
  $G_{Fe:Cr:Cr}^{y}$ *and* $G_{Fe:Cr:Fe}^{y}$

- $G_{Fe:Cr:Cr}^{y}$, $G_{Fe:Cr:Fe}^{y}$ and V1 assessed using *calculated* POP file

The σ Phase

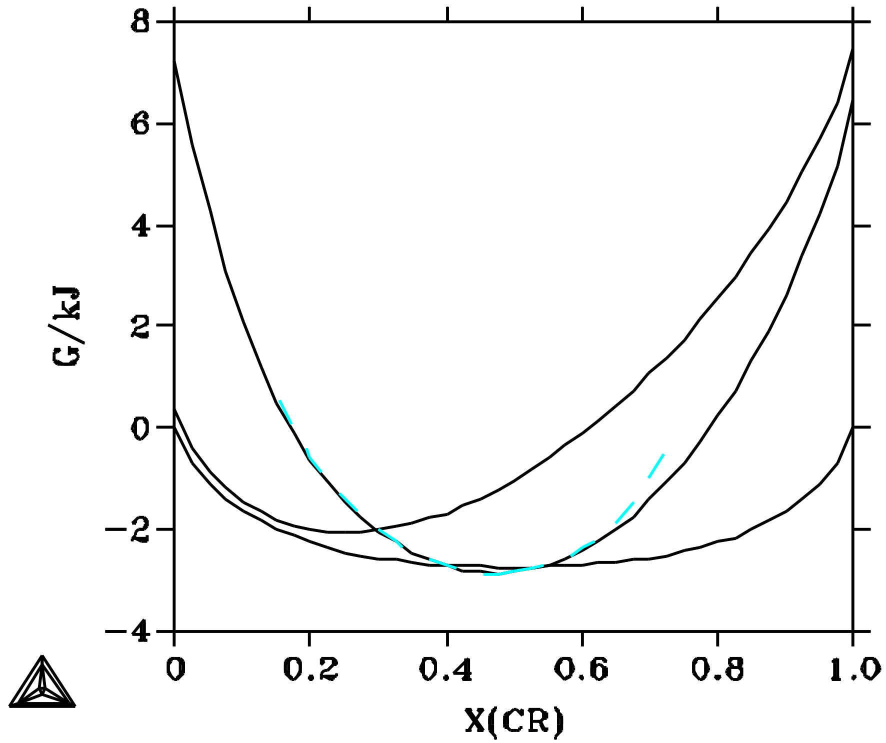


The σ Phase

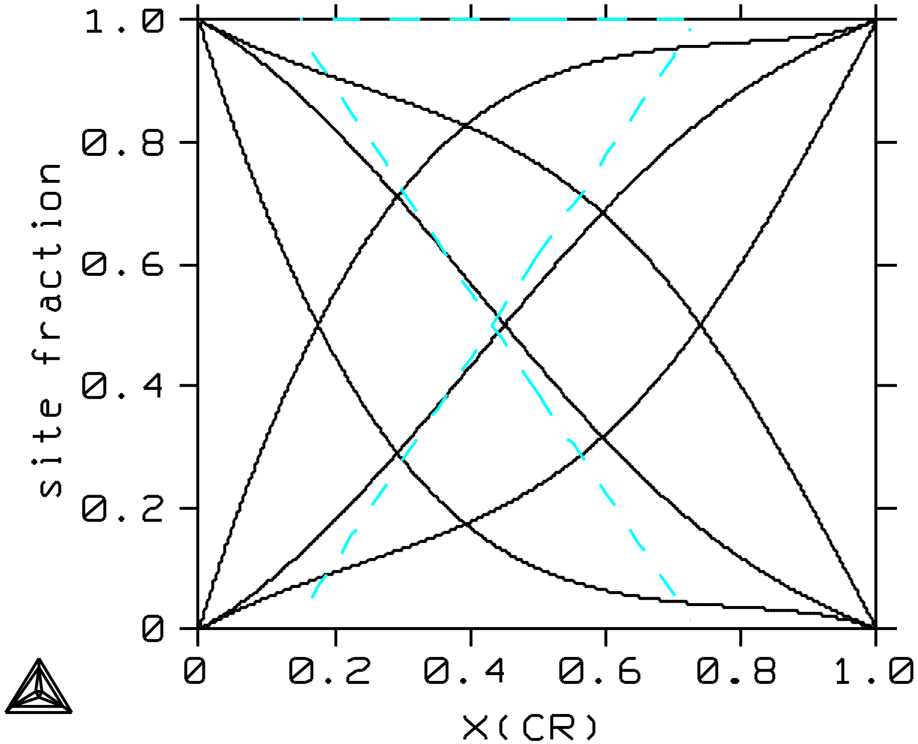


1200
1100
1000
900
800
700
600
500
400
T/K
0
0.2
0.4
0.6
0.8
1.0
x(Cr)
Fe10Cr4Fe16
Cr10Fe4Fe16
Cr10Cr4Fe16
Fe10Fe4Cr16
Fe10Cr4Cr16
Cr10Fe4Cr16

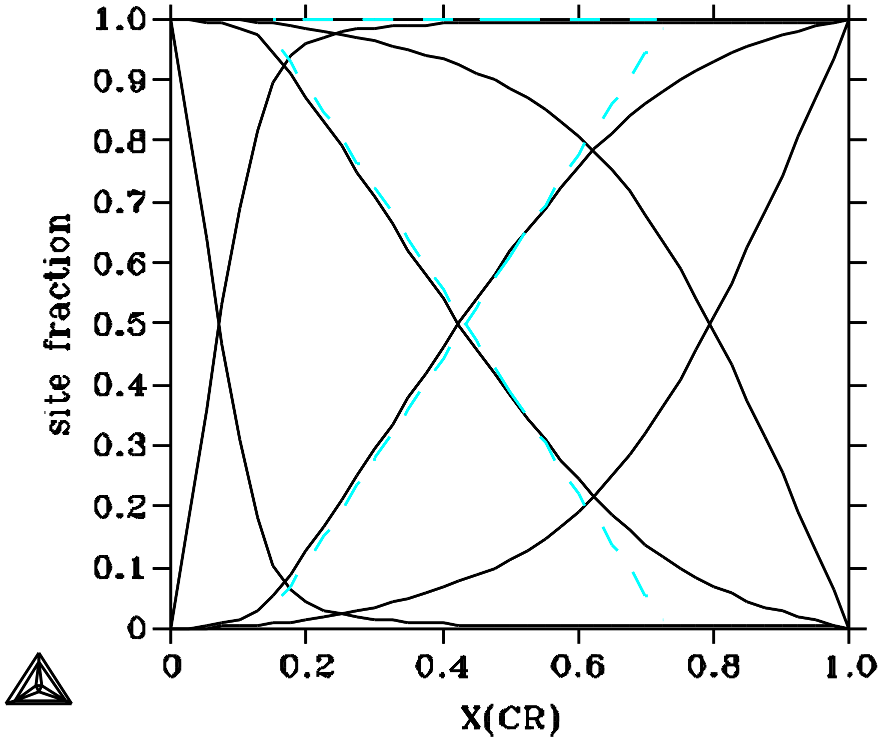
The σ Phase



The σ Phase



The σ Phase



SIGMA

EXCESS MODEL IS REDLICH-KISTER_MUGGIANU

3 SUBLATTICES, SITES 8: 4: 18

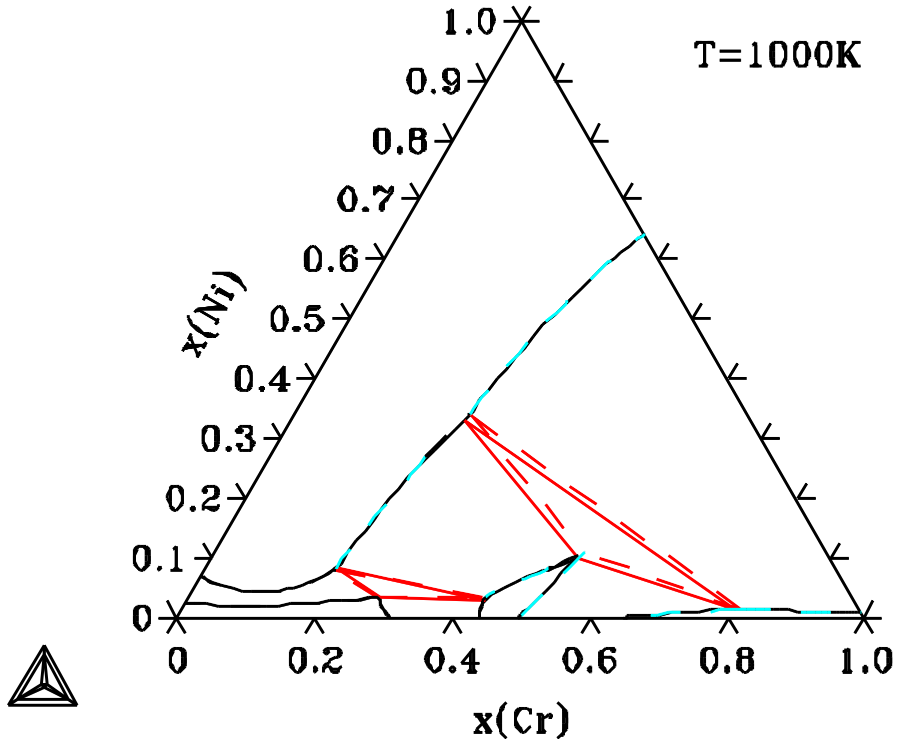
CONSTITUENTS: FE,NI : CR : CR,FE,NI

G(SIGMA,FE:CR:CR;0)- 22 H298(BCC_A2,CR;0)- 8 H298(BCC_A2,FE;0) =
+8*GFEFCC+22*GHSERCR+92300-95.96*T+GPSIG1
G(SIGMA,NI:CR:CR;0)- 22 H298(BCC_A2,CR;0)- 8 H298(FCC_A1,NI;0) =
+8*GHSERNI+22*GHSERCR+221157-227*T
G(SIGMA,FE:CR:FE;0)- 4 H298(BCC_A2,CR;0)- 26 H298(BCC_A2,FE;0) =
+8*GFEFCC+4*GHSERCR+18*GHSERFE+117300-95.96*T+GPSIG2
G(SIGMA,NI:CR:FE;0)- 4 H298(BCC_A2,CR;0)- 18 H298(BCC_A2,FE;0)- 8
H298(FCC_A1,NI;0) = +8*GHSERNI+4*GHSERCR+18*GHSERFE
G(SIGMA,FE:CR:NI;0)- 4 H298(BCC_A2,CR;0)- 8 H298(BCC_A2,FE;0)- 18
H298(FCC_A1,NI;0) = +8*GFEFCC+4*GHSERCR+18*GNIBCC
G(SIGMA,NI:CR:NI;0)- 4 H298(BCC_A2,CR;0)- 26 H298(FCC_A1,NI;0) =
+8*GHSERNI+4*GHSERCR+18*GNIBCC+175400

SIGMA
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
3 SUBLATTICES, SITES 8: 4: 18
CONSTITUENTS: FE,NI : CR : CR,FE,NI

G(SIGMA,FE:CR:CR;0)- 22 H298(BCC_A2,CR;0)- 8 H298(BCC_A2,FE;0) =
+8*GFEFCC+22*GHSERCR+92300-95.96*T+GPSIG1
G(SIGMA,NI:CR:CR;0)- 22 H298(BCC_A2,CR;0)- 8 H298(FCC_A1,NI;0) =
+8*GHSERNI+22*GHSERCR
G(SIGMA,FE:CR:FE;0)- 4 H298(BCC_A2,CR;0)- 26 H298(BCC_A2,FE;0) =
+8*GFEFCC+4*GHSERCR+18*GHSERFE+117300-95.96*T+GPSIG2
G(SIGMA,NI:CR:FE;0)- 4 H298(BCC_A2,CR;0)- 18 H298(BCC_A2,FE;0)- 8
H298(FCC_A1,NI;0) = +8*GHSERNI+4*GHSERCR+18*GHSERFE
G(SIGMA,FE:CR:NI;0)- 4 H298(BCC_A2,CR;0)- 8 H298(BCC_A2,FE;0)- 18
H298(FCC_A1,NI;0) = +8*GFEFCC+4*GHSERCR+18*GNIBCC
G(SIGMA,NI:CR:NI;0)- 4 H298(BCC_A2,CR;0)- 26 H298(FCC_A1,NI;0) =
+8*GHSERNI+4*GHSERCR+18*GNIBCC

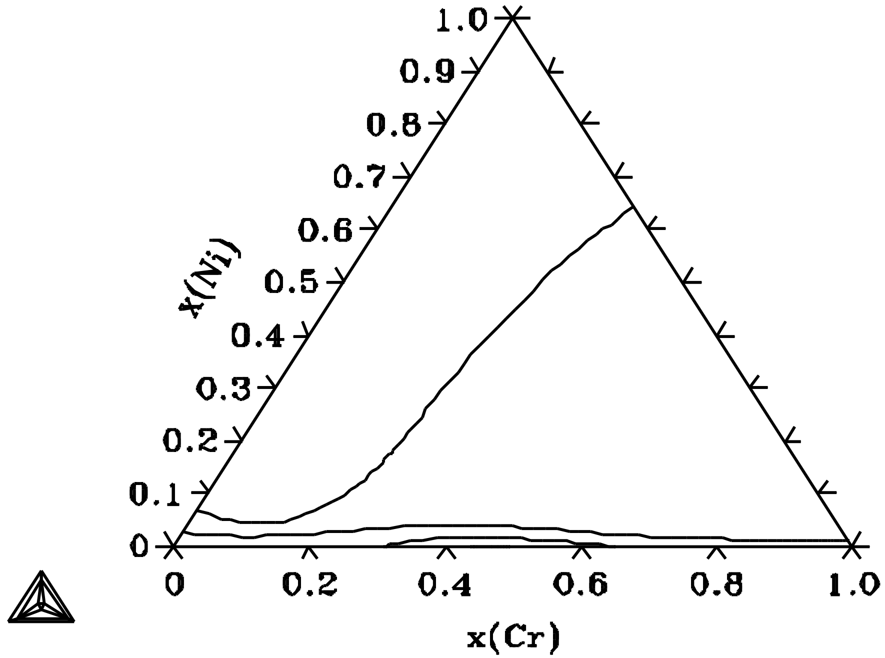
The σ Phase



SIGMA
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
3 SUBLATTICES, SITES 8: 4: 18
CONSTITUENTS: FE,NI : CR : CR,FE,NI

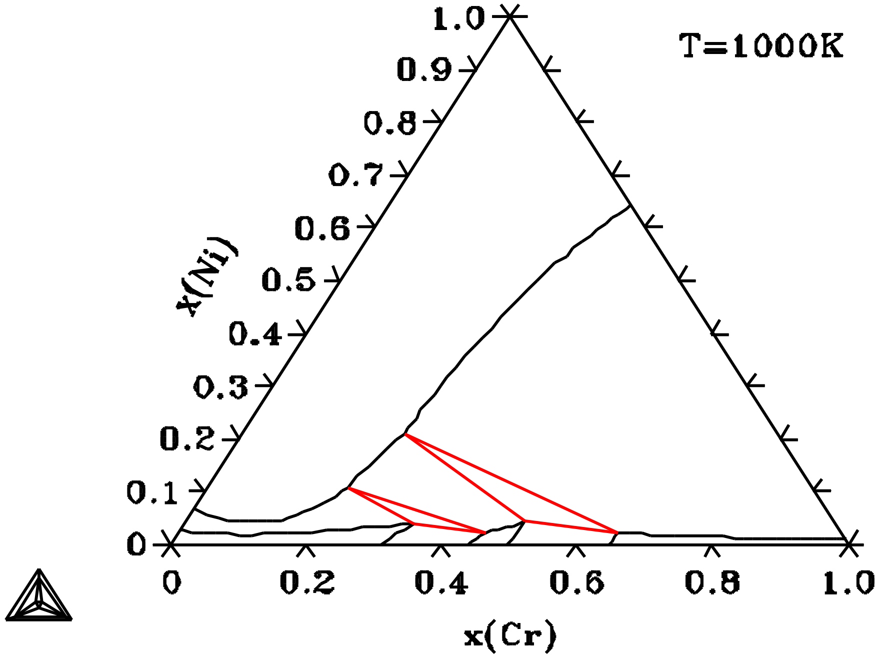
G(SIGMA,FE:CR:CR;0)- 22 H298(BCC_A2,CR;0)- 8 H298(BCC_A2,FE;0) =
+8*GFEFCC+22*GHSERCR+92300-95.96*T+GPSIG1
G(SIGMA,NI:CR:CR;0)- 22 H298(BCC_A2,CR;0)- 8 H298(FCC_A1,NI;0) =
0
G(SIGMA,FE:CR:FE;0)- 4 H298(BCC_A2,CR;0)- 26 H298(BCC_A2,FE;0) =
+8*GFEFCC+4*GHSERCR+18*GHSERFE+117300-95.96*T+GPSIG2
G(SIGMA,NI:CR:FE;0)- 4 H298(BCC_A2,CR;0)- 18 H298(BCC_A2,FE;0)- 8
0
G(SIGMA,FE:CR:NI;0)- 4 H298(BCC_A2,CR;0)- 8 H298(BCC_A2,FE;0)- 18
H298(FCC_A1,NI;0) = 0
G(SIGMA,NI:CR:NI;0)- 4 H298(BCC_A2,CR;0)- 26 H298(FCC_A1,NI;0) =
0

The σ Phase



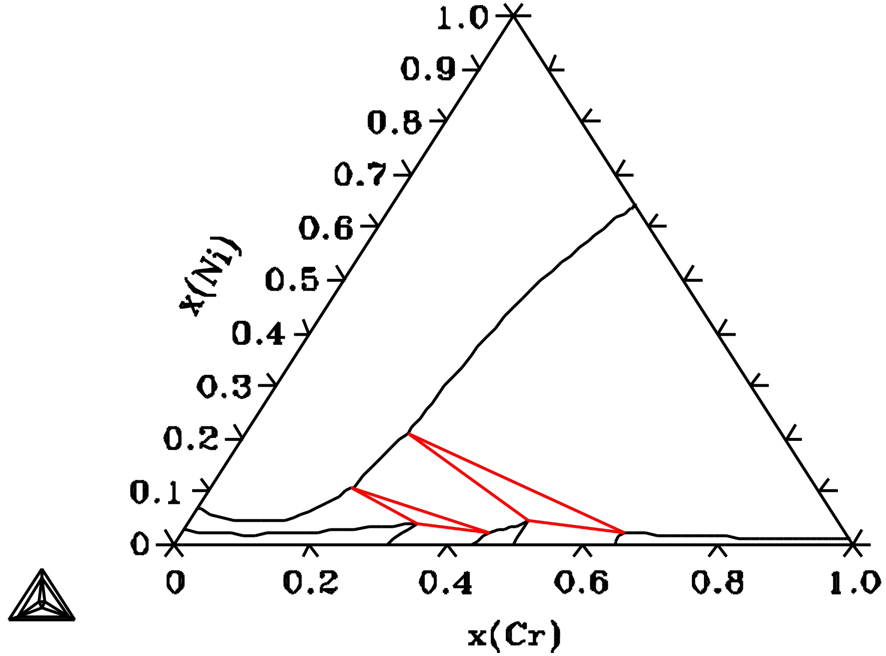
The σ Phase

$$G^{\circ}_{Ni} = 1000 + G^{fcc}_{Ni}$$



The σ Phase

$$G^{\circ}_{Ni} = 10000 + G^{fcc}_{Ni}$$



Conclusions and perspectives

C15 : decrease of the number of parameter

μ and σ phases :

- **new modelling more physicall**
- **not many parameters to be assessed !**
- **need of lattice stability for pure elements**

Database for multicomponent systems

- **less parameters**
- **better extrapolation ?**

C14, C15

Conclusions and perspectives

Implemented in ThermoCalc version N