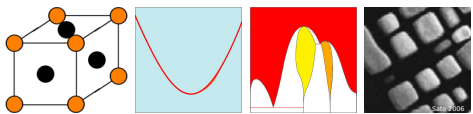
Tomorrow fcc ordering model

Nathalie Dupin

Calcul Thermodynamique

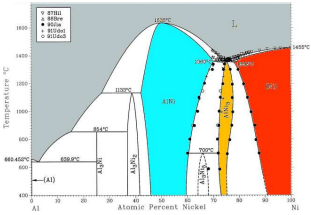
2020 February 24

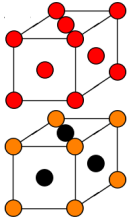
TMS 2020, San Diego, California, USA



Introduction

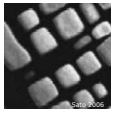
H. Okamoto, 1993

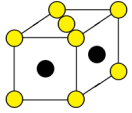




A1
Au

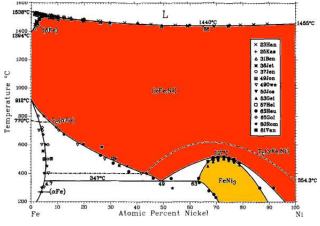
$L1_2$
Cu_3Au



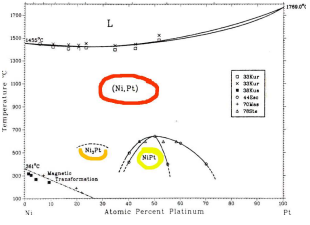


$L1_0$
CuAu

L.J. Swartzendruber, V.P. Itkin, C.B. Alcock, 1991

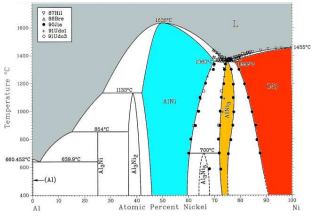


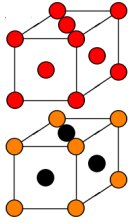
P. Nash and M.F. Singleton, 1991



Introduction

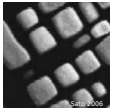
H. Okamoto, 1993

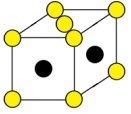




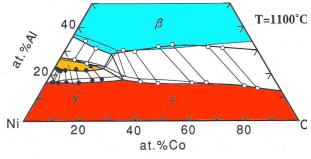
A1
Au

$L1_2$
Cu_3Au

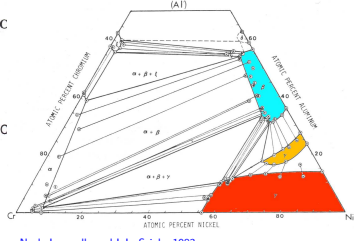




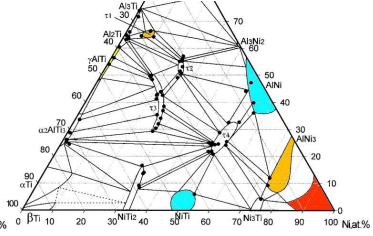
$L1_0$
CuAu



R. Kainuma *et al.*, 1996



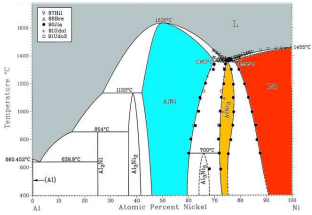
N. de Lanerolle and L.L. Seigle, 1983

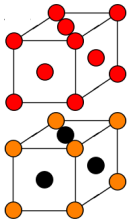


B. Huneau *et al.*, 1999

Introduction

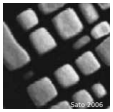
H. Okamoto, 1993

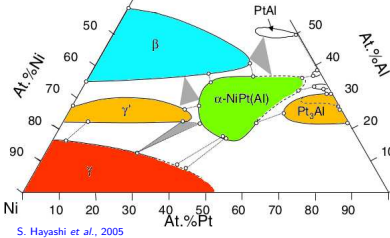




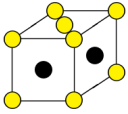
A1
Au

$L1_2$
Cu_3Au

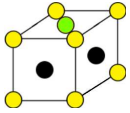




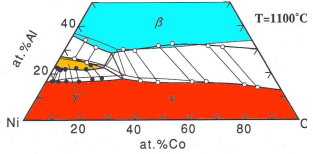
S. Hayashi *et al.*, 2005



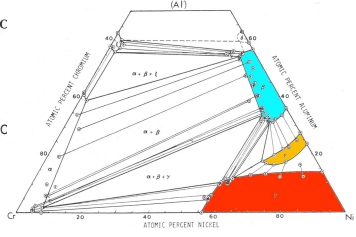
$L1_0$
CuAu



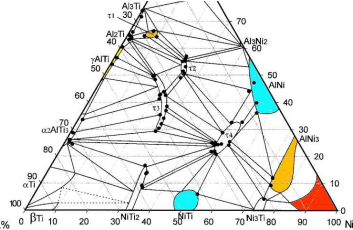
$L6_0$
$CuTi_3$



R. Kainuma *et al.*, 1996



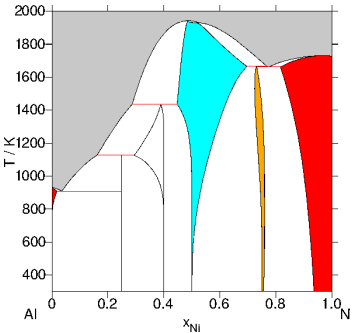
N. de Lanerolle and L.L. Seigle, 1983



B. Huneau *et al.*, 1999

Order-Disorder 2SL CEF

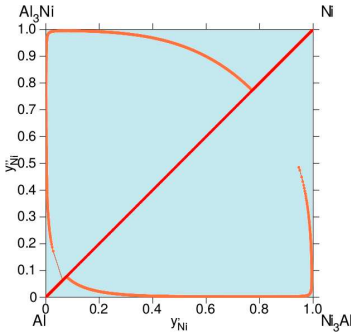
I. Ansara, B. Sundman and P. Willemin, Acta metall., 36 (1988), 977



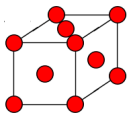
CEF $(Al,Ni)_3(Al,Ni)$
to model γ and γ'
constraints to ensure $(dG = 0)_{y_i' = y_i''}$

Order-Disorder 2SL CEF

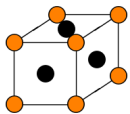
I. Ansara, B. Sundman and P. Willemin, Acta metall., 36 (1988), 977



CEF $(Al,Ni)_3(Al,Ni)$
to model γ and γ'
constraints to ensure $(dG = 0)_{y_i' = y_i''}$



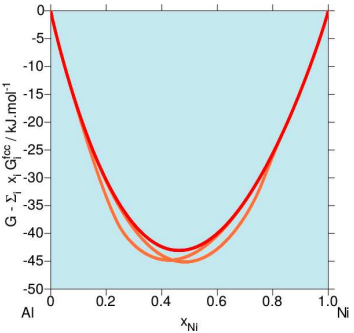
$y_i' = y_i''$



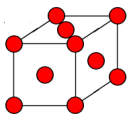
$y_i' \neq y_i''$

Order-Disorder 2SL CEF

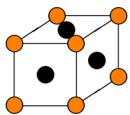
I. Ansara, B. Sundman and P. Willemin, Acta metall., 36 (1988), 977



CEF $(Al,Ni)_3(Al,Ni)$
to model γ and γ'
constraints to ensure $(dG = 0)_{y_i' = y_i''}$



$y_i' = y_i''$



$y_i' \neq y_i''$

Order-Disorder 2SL CEF

I. Ansara, B. Sundman and P. Willemin, Acta metall., 36 (1988), 977

$$G(\text{f.c.c., Al:Ni}) = u_1 + 3L0/16 + 6L1/64$$

$$G(\text{f.c.c., Ni:Al}) = u_2 + 3L0/16 - 6L1/64$$

$$G(\text{f.c.c., Al, Ni:Al; 0}) = 3u_1 + u_2/2 + u_3 + 9L0/16 + 27L1/64$$

$$G(\text{f.c.c., Al, Ni:Ni; 0}) = u_1/2 + 3u_2 + 3u_3 + 9L0/16 - 27L1/64$$

$$G(\text{f.c.c., Al:Al, Ni; 0}) = u_2/2 + u_3 + L0/16 + 9L1/64$$

$$G(\text{f.c.c., Ni:Al, Ni; 0}) = u_1/2 + u_3 + L0/16 - 9L1/64$$

$$G(\text{f.c.c., Al, Ni:Al; 1}) = 3u_4 + 27L1/64$$

$$G(\text{f.c.c., Al, Ni:Ni; 1}) = 3u_5 + 27L1/64$$

$$G(\text{f.c.c., Al:Al, Ni; 1}) = u_4 + L1/64$$

$$G(\text{f.c.c., Ni, Al:Ni; 1}) = u_5 + L1/64$$

G(FCC, AL:AL; 0) − G(FCC, AL; 0) = 0.0
G(FCC, NI; AL; 0) − 0.25 G(FCC, AL; 0) − 0.75 G(FCC, NI; 0) = −40567.2642 + 6.59677•T
G(FCC, AL:NI; 0) − 0.75 G(FCC, AL; 0) − 0.25 G(FCC, NI:0) = −36728.1577 − 1.6322356•T
G(FCC, NI:NI; 0) − G(FCC.NI; 0) = 0.0
G(FCC, AL, NI:AL:0) = −68657.4326 − 13.5507302•T
G(FCC, AL, NI:AL; 1) = +16554.1328 − 18.5152662•T
G(FCC, AL:AL, NI; 0) = +2879.32996-6.17175537•T
G(FCC, AL:AL, NI; 1) = +2958.63986 − .685750611•T
G(FCC, NI:AL, NI; 0) = −2879.33035 + 6.17175537•T
G(FCC, NI:AL, NI; 1) = +2958.63895 − .685575061•T
G(FCC, AL, NI:NI; 0) = −85933.4102 + 23.4798021•T
G(FCC, AL, NI:NI; 1) = +16554.1301 − 18.5152662•T

Split Order-Disorder 2SL CEF

88Ans: Extract of a TDB file from 1991

```
 FCC_A1
$ THIS PHASE IS THE DISORDERED PART OF L12_FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
  2 SUBLATTICES, SITES  1:  1
    CONSTITUENTS: AL,NI : VA

      G(FCC_A1,AL:VA;0)-H298(FCC_A1,AL;0) = +GHSERAL
      G(FCC_A1,NI:VA;0)-H298(FCC_A1,NI;0) = +GHSERNI
      TC(FCC_A1,NI:VA;0) = +633
      BMAGN(FCC_A1,NI:VA;0) = +.52
      L(FCC_A1,AL,NI:VA;0) = +8*U1ALNI
      L(FCC_A1,AL,NI:VA;1) = +4*U4ALNI+64*L1ALNI


U1ALNI   -19323.855+1.241134*T
U4ALNI   +2638.7143
L1ALNI   +319.92555-.6857506*T
```

```
 L12_FCC
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
  3 SUBLATTICES, SITES  .75:  .25:  1
    CONSTITUENTS: AL,NI : AL,NI : VA

      G(L12_FCC,AL:AL:VA;0) =  0.0
      G(L12_FCC,NI:AL:VA;0) = +2*U1ALNI
      G(L12_FCC,AL:NI:VA;0) = +2*U1ALNI
      G(L12_FCC,NI:NI:VA;0) =  0.0
      L(L12_FCC,AL,NI:AL:VA;0) = +4*U1ALNI
      L(L12_FCC,AL,NI:AL:VA;1) = +3*U4ALNI
      L(L12_FCC,AL:AL,NI:VA;0) =  0.0
      L(L12_FCC,AL:AL,NI:VA;1) = +U4ALNI
      L(L12_FCC,AL,NI:NI:VA;0) = +4*U1ALNI
      L(L12_FCC,AL,NI:NI:VA;1) = +3*U4ALNI
      L(L12_FCC,NI:AL,NI:VA;0) =  0.0
      L(L12_FCC,NI:AL,NI:VA;1) = +U4ALNI
```

New implementation splitting G into

- ⇝ a disordered and an ordered contribution
- ⇝ automatically combined by the software.

Split Order-Disorder 2SL CEF

I. Ansara, N. Dupin, H. L. Lukas and B. Sundman, J. Alloys Compounds, 247 (1997), 20

$$G_m = G_m^{dis}(x_i) + G_m^{ord}(y_i', y_i'') - G_m^{ord}(x_i)$$

corresponding to a disordered phase. Hence, the parameters of both ordered and disordered phases can be evaluated independently. This equation has been implemented in

$${}^0L^{\text{f.c.c.-A1}}_{\text{Al,Ni}} = -162\,407.750 + 16.212965T$$
$${}^1L^{\text{f.c.c.-A1}}_{\text{Al,Ni}} = 73\,417.798 - 34.914000T$$
$${}^2L^{\text{f.c.c.-A1}}_{\text{Al,Ni}} = 33\,471.014 - 9.837000T$$
$${}^3L^{\text{f.c.c.-A1}}_{\text{Al,Ni}} = -30\,758.010 + 10.253000T$$

$$u_{1\text{Al,Ni}} = -13415.515 + 2.0819247T$$
$$u_{4\text{Al,Ni}} = 7088.736 - 3.6868954T$$

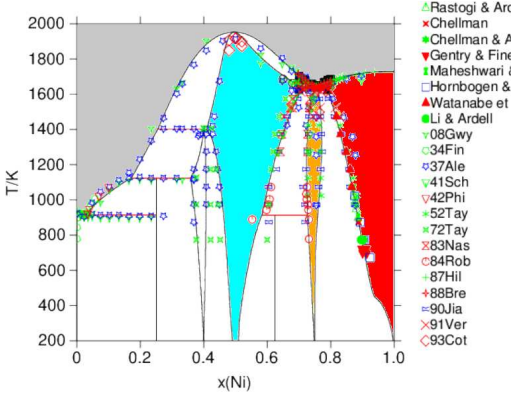
$${}^\circ G^{L1_2}_{\text{Ni:Al}} - 0.75\,{}^\circ G^{\text{f.c.c.-A1}}_{\text{Ni}} - 0.25\,{}^\circ G^{\text{f.c.c.-A1}}_{\text{Al}} = 3u_{1\text{Al,Ni}}$$
$${}^\circ G^{L1_2}_{\text{Al:Ni}} - 0.75\,{}^\circ G^{\text{f.c.c.-A1}}_{\text{Al}} - 0.25\,{}^\circ G^{\text{f.c.c.-A1}}_{\text{Ni}} = 3u_{1\text{Al,Ni}}$$
$${}^0L^{L1_2}_{\text{Al,Ni:Al}} = 6u_{1\text{Al,Ni}}$$
$${}^0L^{L1_2}_{\text{Al,Ni:Ni}} = 6u_{1\text{Al,Ni}}$$
$${}^1L^{L1_2}_{\text{Al,Ni:Al}} = 3u_{4\text{Al,Ni}}$$
$${}^1L^{L1_2}_{\text{Al,Ni:Ni}} = 3u_{4\text{Al,Ni}}$$
$${}^1L^{L1_2}_{\text{Al:Al,Ni}} = u_{4\text{Al,Ni}}$$
$${}^1L^{L1_2}_{\text{Ni:Al,Ni}} = u_{4\text{Al,Ni}}$$

Split Order-Disorder 2SL CEF

I. Ansara, N. Dupin, H. L. Lukas and B. Sundman, J. Alloys Compounds, 247 (1997), 20

$$G_m = G_m^{dis}(x_i) + G_m^{ord}(y_i', y_i'') - G_m^{ord}(x_i)$$

corresponding to a disordered phase. Hence, the parameters of both ordered and disordered phases can be evaluated independently. This equation has been implemented in



$${}^{\circ}G^{L1_2}_{Ni:Al} - 0.75\,{}^{\circ}G^{f.c.c.-A1}_{Ni} - 0.25\,{}^{\circ}G^{f.c.c.-A1}_{Al} = 3u_{1Al,Ni}$$

$${}^{\circ}G^{L1_2}_{Al:Ni} - 0.75\,{}^{\circ}G^{f.c.c.-A1}_{Al} - 0.25\,{}^{\circ}G^{f.c.c.-A1}_{Ni} = 3u_{1Al,Ni}$$

$${}^{0}L^{L1_2}_{Al,Ni:Al} = 6u_{1Al,Ni}$$

$${}^{0}L^{L1_2}_{Al,Ni:Ni} = 6u_{1Al,Ni}$$

$${}^{1}L^{L1_2}_{Al,Ni:Al} = 3u_{4Al,Ni}$$

$${}^{1}L^{L1_2}_{Al,Ni:Ni} = 3u_{4Al,Ni}$$

$${}^{1}L^{L1_2}_{Al:Al,Ni} = u_{4Al,Ni}$$

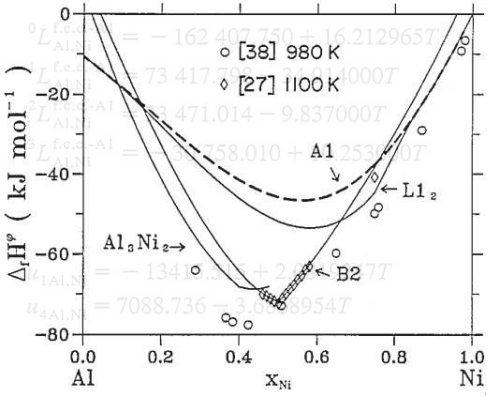
$${}^{1}L^{L1_2}_{Ni:Al,Ni} = u_{4Al,Ni}$$

Split Order-Disorder 2SL CEF

I. Ansara, N. Dupin, H. L. Lukas and B. Sundman, J. Alloys Compounds, 247 (1997), 20

$$G_m = G_m^{dis}(x_i) + G_m^{ord}(y_i', y_i'') - G_m^{ord}(x_i)$$

corresponding to a disordered phase. Hence, the parameters of both ordered and disordered phases can be evaluated independently. This equation has been implemented in



$$^{\circ}G^{L1_2}_{Ni:Al} - 0.75\,^{\circ}G^{f.c.c.\text{-}A1}_{Ni} - 0.25\,^{\circ}G^{f.c.c.\text{-}A1}_{Al} = 3u_{1Al,Ni}$$

$$^{\circ}G^{L1_2}_{Al:Ni} - 0.75\,^{\circ}G^{f.c.c.\text{-}A1}_{Al} - 0.25\,^{\circ}G^{f.c.c.\text{-}A1}_{Ni} = 3u_{1Al,Ni}$$

$$^{0}L^{L1_2}_{Al,Ni:Al} = 6u_{1Al,Ni}$$

$$^{0}L^{L1_2}_{Al,Ni:Ni} = 6u_{1Al,Ni}$$

$$^{1}L^{L1_2}_{Al,Ni:Al} = 3u_{4Al,Ni}$$

$$^{1}L^{L1_2}_{Al,Ni:Ni} = 3u_{4Al,Ni}$$

$$^{1}L^{L1_2}_{Al:Al,Ni} = u_{4Al,Ni}$$

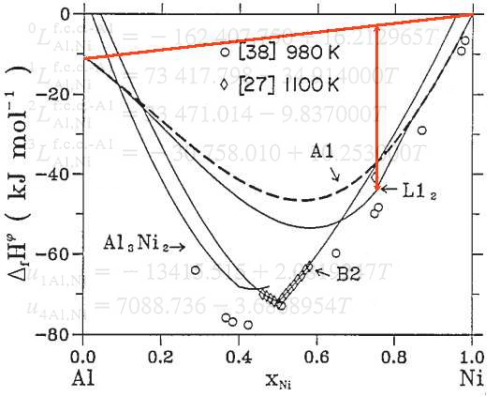
$$^{1}L^{L1_2}_{Ni:Al,Ni} = u_{4Al,Ni}$$

Split Order-Disorder 2SL CEF

I. Ansara, N. Dupin, H. L. Lukas and B. Sundman, J. Alloys Compounds, 247 (1997), 20

$$G_m = G_m^{dis}(x_i) + G_m^{ord}(y_i', y_i'') - G_m^{ord}(x_i)$$

corresponding to a disordered phase. Hence, the parameters of both ordered and disordered phases can be evaluated independently. This equation has been implemented in



$$^{\circ}G^{L1_2}_{Ni:Al} - 0.75\,^{\circ}G^{f.c.c.-A1}_{Ni} - 0.25\,^{\circ}G^{f.c.c.-A1}_{Al} = 3u_{1Al,Ni}$$

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$$^{0}L^{L1_2}_{Al,Ni:Al} = 6u_{1Al,Ni}$$

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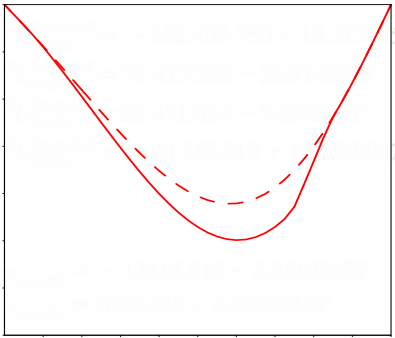
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Split Order-Disorder 2SL CEF

I. Ansara, N. Dupin, H. L. Lukas and B. Sundman, J. Alloys Compounds, 247 (1997), 20

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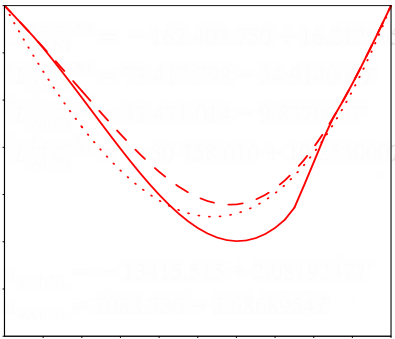
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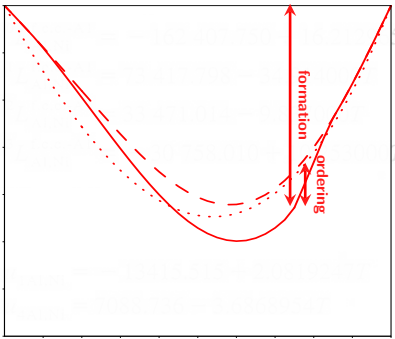
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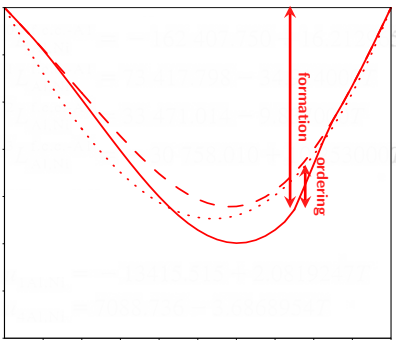
The meaning of `G(L12,NI:AL;0)` depends on the constraints imposed to the parameters of the ordered contribution. It can be

- ⇝ the formation energy of the stoichiometric compound from the elements if $G_m^{ord}(x_i) = G_m^{dis}(x_i)$,
- ⇝ its ordering energy from the disordered alloy if $G_m^{ord}(x_i) = 0$,
- ⇝ or any other meaningless value.

Split Order-Disorder 2SL CEF

I. Ansara, N. Dupin, H. L. Lukas and B. Sundman, J. Alloys Compounds, 247 (1997), 20

$$G_m = G_m^{dis}(x_i) + G_m^{ord}(y_i', y_i'') - G_m^{ord}(x_i)$$



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Actually, the ordered and disordered phases cannot be assessed fully independly. If the disordered phase is fixed, some energies and configurations will be forbidden for the ordered state.

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OD L12-2SL = OD 4SL

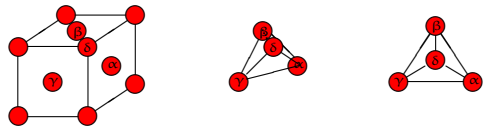
N. Dupin, Thesis Grenoble 1995
N. Dupin, B. Sundman, Scand. J. Metall., 30, 184-192 (2001).

When coming to ternary systems, the constraints obtained from $(dG = 0)_{y_i' = y_i''}$ showed limitations.

A new approach using the equivalence to a 4SL model has then been setup.

OD L12-2SL = OD 4SL

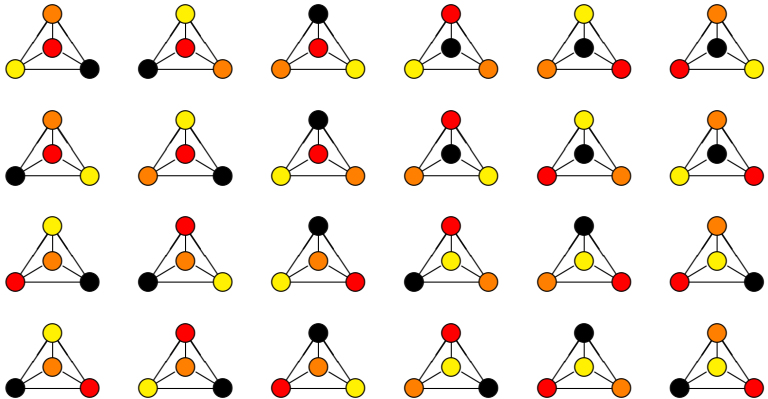
The fcc lattice is built on regular tetrahedra.



same occupation on the 4SL $\Rightarrow$ the disorder ($A1$)

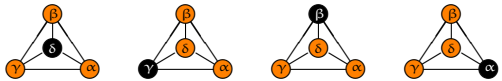
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From the symmetry of the regular tetrahedra, the following configurations are equivalent.
Considering this symmetry for all the thermodynamic parameters makes the 4SL be OD.



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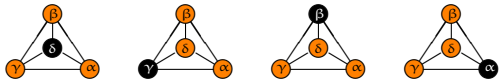


$L1_2$ configurations : 3 SL have the same occupation

$$G^{4SL}_{A:A:A:B} = G^{4SL}_{A:A:B:A} = G^{4SL}_{A:B:A:A} = G^{4SL}_{B:A:A:A}$$

OD L12-2SL = OD 4SL

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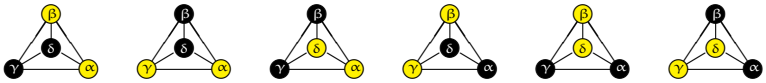
$$G^{4SL}_{A:A:A:B} = G^{4SL}_{A:A:B:A} = G^{4SL}_{A:B:A:A} = G^{4SL}_{B:A:A:A}$$

Also standing for excess parameters

$$L^{4SL}_{AB:*:*:*} = L^{4SL}_{*:AB:*:*} = L^{4SL}_{*:*:AB:*} = L^{4SL}_{*:*:*:AB}$$

OD L12-2SL = OD 4SL

From the symmetry of the regular tetrahedra, the following configurations are equivalent.
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$L1_0$ configurations

$$G^{4SL}_{A:A:B:B} = G^{4SL}_{A:B:A:B} = G^{4SL}_{A:B:B:A} = G^{4SL}_{B:A:A:B} = G^{4SL}_{B:A:B:A} = G^{4SL}_{B:B:A:A}$$

also standing for reciprocal interaction parameters

$$L^{4SL}_{AB:AB:*:*} = L^{4SL}_{AB:*:AB:*} = L^{4SL}_{AB:*:*:AB} = L^{4SL}_{*:AB:AB:*} = L^{4SL}_{*:AB:*:AB} = L^{4SL}_{*:*:AB:AB}$$

OD L12-2SL = OD 4SL

$$G^{2SL} = \sum_i \sum_j y_i^{'} y_j^{''} G_{i;j}^{2SL} + RT\left(3\sum_i y_i^{'} \ln y_i^{'} + \sum_i y_i^{''} \ln y_i^{''}\right) + {}^{xs}G^{2SL}$$

OD L12-2SL = OD 4SL

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$\rightsquigarrow$ 4 $G_{i:j}^{2SL}$: $G_{A_4}^{2SL}$, $G_{A_3B}^{2SL}$, $G_{B_3A}^{2SL}$ and $G_{B_4}^{2SL}$

$\rightsquigarrow$ ${}^{xs}G^{2SL} = y_A^{'} y_B^{'} y_A^{''}\left(L0_{AB:A}^{2SL} + (y_A^{'} - y_B^{'})L1_{AB:A}^{2SL}\right) + y_A^{'} y_B^{'} y_B^{''}\left(L0_{AB:B}^{2SL} + (y_A^{'} - y_B^{'})L1_{AB:B}^{2SL}\right)$

$+ y_A^{'} y_A^{''} y_B^{''}\left(L0_{A:AB}^{2SL} + (y_A^{''} - y_B^{''})L1_{A:AB}^{2SL}\right) + y_B^{'} y_A^{''} y_B^{''}\left(L0_{B:AB}^{2SL} + (y_A^{''} - y_B^{''})L1_{B:AB}^{2SL}\right)$

$+ y_A^{'} y_B^{'} y_A^{''} y_B^{''}\, L_{AB:AB}^{2SL}$

OD L12-2SL = OD 4SL

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$$G^{4SL} = \sum_i \sum_j y_i^{\alpha} y_j^{\beta} y_k^{\gamma} y_l^{\delta} G^{4SL}_{i:j:k:l} + RT\sum_s \sum_i y_i^{s} \ln y_i^{s} + {}^{xs}G^{4SL}$$

OD L12-2SL = OD 4SL

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$\rightsquigarrow$ 16 $G^{4SL}_{i:j:k:l}$, 5 indepedent: $G^{4SL}_{A_4}$, $G^{4SL}_{A_3B}$, $G^{4SL}_{A_2B_2}$, $G^{4SL}_{AB_3}$, $G^{4SL}_{B_4}$

$\rightsquigarrow$ $L0^{4SL}_{AB:*:*:*} = L0^{4SL}_{*:AB:*:*} = L0^{4SL}_{*:*:AB:*} = L0^{4SL}_{*:*:*:AB}$

$L1^{4SL}_{AB:*:*:*} = L1^{4SL}_{*:AB:*:*} = L1^{4SL}_{*:*:AB:*} = L1^{4SL}_{*:*:*:AB}$

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OD L12-2SL = OD 4SL

$$
\begin{aligned}
G^{2SL}_{A_3B} &= G^{4SL}_{A_3B} \\
G^{2SL}_{B_3A} &= G^{4SL}_{AB_3} \\
L0^{2SL}_{AB:A} &= -1.5\,G^{4SL}_{AB_3} + 1.5\,G^{4SL}_{A_2B_2} + 1.5\,G^{4SL}_{A_3B} + 3\,L0^{4SL}_{AB:*:*:*} + 0.75\,L^{4SL}_{AB:AB:*:*} \\
L0^{2SL}_{AB:B} &= +1.5\,G^{4SL}_{AB_3} + 1.5\,G^{4SL}_{A_2B_2} - 1.5\,G^{4SL}_{A_3B} + 3\,L0^{4SL}_{AB:*:*:*} + 0.75\,L^{4SL}_{AB:AB:*:*} \\
L0^{2SL}_{*:AB} &= L0^{4SL}_{AB:*:*:*} \\
L1^{2SL}_{AB:A} &= +0.5\,G^{4SL}_{AB_3} - 1.5\,G^{4SL}_{A_2B_3} + 1.5\,G^{4SL}_{A_3B} + 3\,L1^{4SL}_{AB:*:*:*} \\
L1^{2SL}_{AB:B} &= -1.5\,G^{4SL}_{AB_3} + 1.5\,G^{4SL}_{A_2B_3} - 0.5\,G^{4SL}_{A_3B} + 3\,L1^{4SL}_{AB:*:*:*} \\
L1^{2SL}_{*:AB} &= L1^{4SL}_{AB:*:*:*} \\
L2^{2SL}_{AB:*} &= -0.75\,L^{4SL}_{AB:AB:*:*} \\
L^{2SL}_{AB:AB} &= 3\,L^{4SL}_{AB:AB:*:*}
\end{aligned}
$$

OD L12-2SL = OD 4SL

$$G'_{B:A} = G_{AB_3}$$

$$G'_{A:B} = G_{A_3B}$$

$$L'^{0}_{A,B:A} = -\frac{3}{2}G_{AB_3} + \frac{3}{2}G_{A_2B_2} + \frac{3}{2}G_{A_3B}$$

$$L'^{0}_{A,B:B} = +\frac{3}{2}G_{AB_3} + \frac{3}{2}G_{A_2B_2} - \frac{3}{2}G_{A_3B}$$

$$L'^{1}_{A,B:A} = +\frac{1}{2}G_{AB_3} - \frac{3}{2}G_{A_2B_2} + \frac{3}{2}G_{A_3B}$$

$$L'^{1}_{A,B:B} = +\frac{3}{2}G_{AB_3} + \frac{3}{2}G_{A_2B_2} - \frac{1}{2}G_{A_3B}$$

$$L'^{0}_{*,A,B} = L'^{0}_{A,B}$$

$$L'^{1}_{*,A,B} = L'^{1}_{A,B}$$

$$L'^{0}_{A,B,*} = 3L'^{0}_{A,B}$$

$$L'^{1}_{A,B,*} = 3L'^{1}_{A,B}$$

$$\begin{aligned} L'^{0}_{A,B,C:A} = &+G_{AB_3} - \frac{3}{2}G_{A_2B_2} - \frac{3}{2}G_{A_3B} + G_{AC_3} \\ &- \frac{3}{2}G_{A_2C_2} - \frac{3}{2}G_{A_3C} - \frac{3}{2}G_{ABC_2} - \frac{3}{2}G_{AB_2C} \\ &+ 6G_{A_2BC} \end{aligned}$$

$$\begin{aligned} L'^{0}_{A,B,C:B} = &-\frac{3}{2}G_{AB_3} - \frac{3}{2}G_{A_2B_2} + G_{A_3B} + G_{BC_3} \\ &- \frac{3}{2}G_{B_2C_2} - \frac{3}{2}G_{B_3C} - \frac{3}{2}G_{ABC_2} + 6G_{AB_2C} \\ &- \frac{3}{2}G_{A_2BC} \end{aligned}$$

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$$L'^{0}_{A,B,C:C} = -\frac{3}{2}G_{A_3C} - \frac{3}{2}G_{B_3C} + \frac{3}{2}G_{AB_2C} + \frac{3}{2}G_{A_2BC}$$

$$L'^{0}_{A,C,B:B} = -\frac{3}{2}G_{A_3B} - \frac{3}{2}G_{BC_3} + \frac{3}{2}G_{ABC_2} + \frac{3}{2}G_{A_2BC}$$

$$L'^{0}_{B,C,A:A} = -\frac{3}{2}G_{AB_3} - \frac{3}{2}G_{AC_3} + \frac{3}{2}G_{ABC_2} + \frac{3}{2}G_{AB_2C}$$

$$L'^{1}_{A,B,C:C} = -\frac{1}{2}G_{A_3C} + \frac{1}{2}G_{B_3C} - \frac{3}{2}G_{AB_2C} + \frac{3}{2}G_{A_2BC}$$

$$L'^{1}_{A,C,B:B} = -\frac{1}{2}G_{A_3B} + \frac{1}{2}G_{BC_3} - \frac{3}{2}G_{ABC_2} + \frac{3}{2}G_{A_2BC}$$

$$L'^{1}_{B,C,A:A} = -\frac{1}{2}G_{AB_3} + \frac{1}{2}G_{AC_3} - \frac{3}{2}G_{ABC_2} + \frac{3}{2}G_{AB_2C}$$

$$\begin{aligned} L'^{0}_{A,B,C:D} = &\ G_{A_3D} + G_{B_3D} + G_{C_3D} - \frac{3}{2}G_{AB_2D} - \frac{3}{2}G_{A_2BD} \\ &- \frac{3}{2}G_{AC_2D} - \frac{3}{2}G_{BC_2D} - \frac{3}{2}G_{A_2CD} - \frac{3}{2}G_{B_2CD} \\ &+ 6G_{A_2CD} \end{aligned}$$

$$\begin{aligned} L'^{0}_{A,B,D:C} = &\ G_{A_3C} + G_{B_3C} + G_{CD_3} - \frac{3}{2}G_{AB_2C} - \frac{3}{2}G_{A_2BC} \\ &- \frac{3}{2}G_{ACD_2} - \frac{3}{2}G_{A_2CD} - \frac{3}{2}G_{BCD_2} - \frac{3}{2}G_{B_2CD} \\ &+ 6G_{ABCD} \end{aligned}$$

$$\begin{aligned} L'^{0}_{A,C,D:B} = &\ G_{A_3B} + G_{BC_3} + G_{BD_3} - \frac{3}{2}G_{ABC_2} - \frac{3}{2}G_{A_2BC} \\ &- \frac{3}{2}G_{ABD_2} - \frac{3}{2}G_{A_2BD} - \frac{3}{2}G_{BCD_2} - \frac{3}{2}G_{BC_2D} \\ &+ 6G_{ABCD} \end{aligned}$$

$$\begin{aligned} L'^{0}_{B,C,D:A} = &\ G_{AB_3} + G_{AC_3} + G_{AD_3} - \frac{3}{2}G_{ABC_2} - \frac{3}{2}G_{AB_2C} \\ &- \frac{3}{2}G_{ABD_2} - \frac{3}{2}G_{AB_2D} - \frac{3}{2}G_{ACD_2} - \frac{3}{2}G_{AC_2D} \\ &+ 6G_{ABCD} \end{aligned}$$

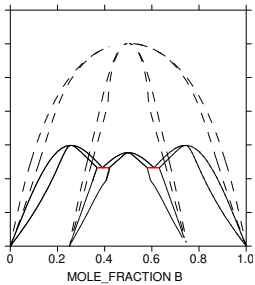
Even if a rather limited amount of independent variables is used, many interaction parameters, in every binary, ternary and quaternary systems, have to be written in order to allow the disordered state.

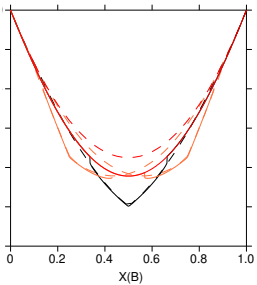
They are heavy to handle for human database managers.

They consume computational time.

Would it be possible to work directely with a wild 4SL model?

OD 4SL CEF





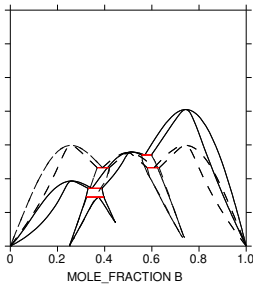
$$G = \sum_i \sum_j \sum_k \sum_l y_i^\alpha y_j^\beta y_k^\gamma y_l^\delta G_{ijkl}$$
$$+ RT \sum_s \sum_i \frac{1}{4} y_i^s \ln y_i^s$$
$$+ \sum_s \sum_{r>s} y_A^s y_B^s L_{AB:*:*:*}$$
$$+ \sum_s \sum_{r>s} y_A^s y_B^s y_A^r y_B^r L_{AB:AB:*:*}$$

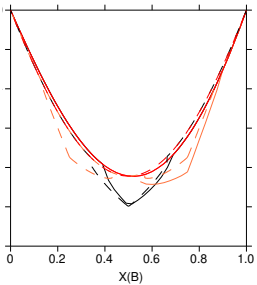
with $\epsilon_{AB} = \frac{1}{3} G_{A3B} = \frac{1}{3} G_{AB3} = \frac{1}{4} G_{A2B2}$

$L_{AB:AB:*:*} = 0$ (dashed)
$L_{AB:AB:*:*} = \epsilon_{AB}$ (solid)

Reciprocal parameters affect the ordering temperatures and the separation of the ordering maxima. Even for limited effect on the thermodynamics, the phase diagram change is significant. It can describe the effect of sro. It is difficult to assess when the experimental information is available on a reduced range of composition.

OD 4SL CEF





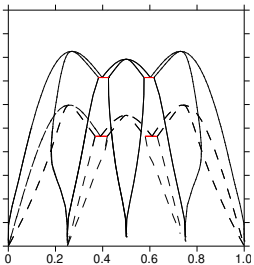
Constant bond energy is in general not in agreement with experimental or DFT results. The asymmetry of the bond energy impacts not only the ordered states but also the disordered phase.

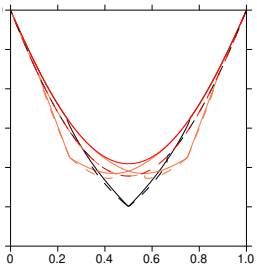
$$G = \sum_i \sum_j \sum_k \sum_l y_i^\alpha y_j^\beta y_k^\gamma y_l^\delta G_{ijkl}$$
$$+ RT \sum_s \sum_i \frac{1}{4} y_i^s \ln y_i^s$$
$$+ \sum_s \sum_{r>s} y_A^s y_B^s L_{AB:*:*:*}$$
$$+ \sum_s \sum_{r>s} y_A^s y_B^s y_A^r y_B^r L_{AB:AB:*:*}$$

with $\epsilon_{AB} = \frac{1}{3} G_{A3B} = \frac{1}{3} G_{AB3} = \frac{1}{4} G_{A2B2}$
for dashed lines

and $G_{A2B2} = 4\epsilon_{AB}$
$G_{AB3} = 3\epsilon_{AB} - 10\%$
$G_{A3B} = 3\epsilon_{AB} + 10\%$
for solid lines

OD 4SL CEF





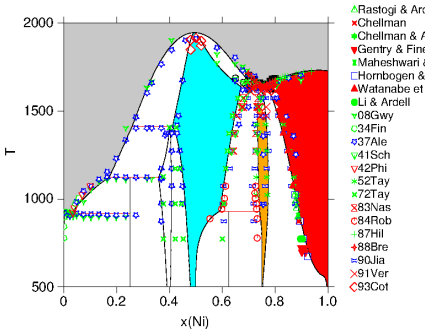
Interaction parameters affect the width of the two phase field. They impact significantly the Gibbs energy of the disordered phase and thus of the ordering energies from the disordered mixture. They describe interactions between further than nearest neighbors. Sub-regular terms can of course also be considered.

$$G = \sum_i \sum_j \sum_k \sum_l y_i^\alpha y_j^\beta y_k^\gamma y_l^\delta G_{ijkl}$$
$$+ RT \sum_s \sum_i \frac{1}{4} y_i^s \ln y_i^s$$
$$+ \sum_s \sum_{r>s} y_A^s y_B^s L_{AB:*:*:*}$$
$$+ \sum_s \sum_{r>s} y_A^s y_B^s y_A^r y_B^r L_{AB:AB:*:*}$$

with $\epsilon_{AB} = \frac{1}{3} G_{A3B} = \frac{1}{3} G_{AB3} = \frac{1}{4} G_{A2B2}$
$L_{AB:*:*:*} = 0$ (dashed)
$L_{AB:*:*:*} = -\epsilon_{AB}$ (solid)

OD 4SL CEF

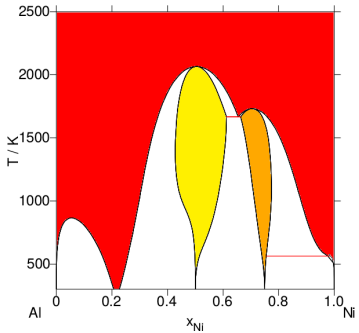
B. Sundman, N. Dupin, JEEP 2003, Lyon

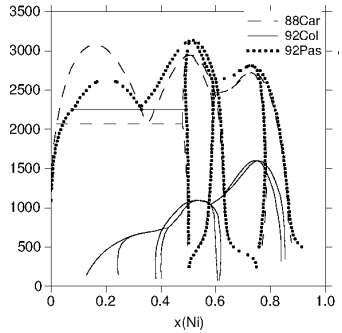


$$G = \sum_i \sum_j \sum_k \sum_l y_i^\alpha y_j^\beta y_k^\gamma y_l^\delta G_{ijkl}$$
$$+ RT \sum_s \sum_i \frac{1}{4} y_i^s \ln y_i^s$$
$$+ \sum_s \sum_{r>s} y_A^s y_B^s L_{AB:*:*:*}$$
$$+ \sum_s \sum_{r>s} y_A^s y_B^s y_A^r y_B^r L_{AB:AB:*:*}$$

OD 4SL CEF

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$$G = \sum_i \sum_j \sum_k \sum_l y_i^\alpha y_j^\beta y_k^\gamma y_l^\delta G_{ijkl}$$

$$+ RT \sum_s \sum_i \frac{1}{4} y_i^s \ln y_i^s$$

$$+ \sum_s \sum_{r>s} y_A^s y_B^s L_{AB:*:*:*}$$

$$+ \sum_s \sum_{r>s} y_A^s y_B^s y_A^r y_B^r L_{AB:AB:*:*}$$

4SL Split in 3 (DIS_PART)

B. Sundman, N. Dupin, JEEP 2003, Lyon

$$G = G^{dis}(x_i) + \Delta G^{ord}(y_i^s) - \Delta G^{ord}(y_i^s = x_i)$$

```
 FCC_A1
$ THIS PHASE IS THE DISORDERED PART OF ORD_FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
 ADDITIONAL CONTRIBUTION FROM MAGNETIC ORDERING
      Magnetic function below Curie Temperature
      +1-.860338755*TAO**(-1)-.17449124*TAO**3-.00775516624*TAO**9
      -.0017449124*TAO**15
      Magnetic function above Curie Temperature
       -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)
      -2.84601512E-04*TAO**(-25)
  2 SUBLATTICES, SITES  1:  1
    CONSTITUENTS: AL,NI : VA

      G(FCC_A1,AL:VA;0)-H298(FCC_A1,AL;0) = +GHSERAL
      G(FCC_A1,NI:VA;0)-H298(FCC_A1,NI;0) = +GHSERNI
      TC(FCC_A1,NI:VA;0) = +633
      BMAGN(FCC_A1,NI:VA;0) = +.52
      TC(FCC_A1,AL,NI:VA;0) = -1112
      TC(FCC_A1,AL,NI:VA;1) = +1745
      L(FCC_A1,AL,NI:VA;0) = +AL3NI+1.5*AL2NI2+ALNI3+1.5*RALNI+4*LOALNI
      L(FCC_A1,AL,NI:VA;1) = +2*AL3NI-2*ALNI3
      L(FCC_A1,AL,NI:VA;2) = +AL3NI-1.5*AL2NI2+ALNI3-1.5*RALNI
```

The interaction parameters in the disordered part are expressed in function of the parameters of the ordered part.

The reference in the ordered part is not explicited.

```
 ORD_FCC
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
  5 SUBLATTICES, SITES  .25:  .25:  .25:  .25:  1
    CONSTITUENTS: AL,NI : AL,NI : AL,NI : AL,NI : VA

      G(ORD_FCC,AL:AL:AL:AL:VA;0) = 0.0
      G(ORD_FCC,NI:AL:AL:AL:VA;0) = +AL3NI
      G(ORD_FCC,AL:NI:AL:AL:VA;0) = +AL3NI
      G(ORD_FCC,NI:NI:AL:AL:VA;0) = +AL2NI2
      G(ORD_FCC,AL:AL:NI:AL:VA;0) = +AL3NI
      G(ORD_FCC,NI:AL:NI:AL:VA;0) = +AL2NI2
      G(ORD_FCC,AL:NI:NI:AL:VA;0) = +AL2NI2
      G(ORD_FCC,NI:NI:NI:AL:VA;0) = +ALNI3
      G(ORD_FCC,AL:AL:AL:NI:VA;0) = +AL3NI
      G(ORD_FCC,NI:AL:AL:NI:VA;0) = +AL2NI2
      G(ORD_FCC,AL:NI:AL:NI:VA;0) = +AL2NI2
      G(ORD_FCC,NI:NI:AL:NI:VA;0) = +ALNI3
      G(ORD_FCC,AL:AL:NI:NI:VA;0) = +AL2NI2
      G(ORD_FCC,NI:AL:NI:NI:VA;0) = +ALNI3
      G(ORD_FCC,AL:NI:NI:NI:VA;0) = +ALNI3
      G(ORD_FCC,NI:NI:NI:NI:VA;0) = 0.0
      L(ORD_FCC,*:*:AL,NI:AL,NI:VA;0) = +URALNI
      L(ORD_FCC,*:AL,NI:*:AL,NI:VA;0) = +URALNI
      L(ORD_FCC,AL,NI:*:*:AL,NI:VA;0) = +URALNI
      L(ORD_FCC,*:AL,NI:AL,NI:*:VA;0) = +URALNI
      L(ORD_FCC,AL,NI:*:AL,NI:*:VA;0) = +URALNI
      L(ORD_FCC,AL,NI:AL,NI:*:*:VA;0) = +URALNI
      L(ORD_FCC,AL,NI:*:*:*:VA;0) = +LOALNI
      L(ORD_FCC,*:AL,NI:*:*:VA;0) = +LOALNI
      L(ORD_FCC,*:*:AL,NI:*:VA;0) = +LOALNI
      L(ORD_FCC,*:*:*:AL,NI:VA;0) = +LOALNI
```

F-4SL Split in 3 (DIS_PART)

$$G = G^{dis}(x_i) + \Delta G^{ord}(y_i^s) - \Delta G^{ord}(y_i^s = x_i)$$

B. Sundman, N. Dupin, JEEP 2003, Lyon

```
 FCC_A1
$ THIS PHASE IS THE DISORDERED PART OF ORD_FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
 ADDITIONAL CONTRIBUTION FROM MAGNETIC ORDERING
  Magnetic Ordering Extra Curie Temperature
   TC:-.860338755*TAO*+(-1)-.17449124*TAO**3-.00775516624*TAO**9
   -.0017449124*TAO**15
  Magnetic Ordering Extra Curie Temperature
   -.0426902268*TAO*+(-5)-.0013552453*TAO**(-15)-.000284601512*TAO**(-25)
  2 SUBLATTICES, SITES  1:  1
    CONSTITUENTS: AL,NI : VA

      G(FCC_A1,AL:VA;0)-H298(FCC_A1,AL;0) = +GHSERAL
      G(FCC_A1,NI:VA;0)-H298(FCC_A1,NI;0) = +GHSERNI
      TC(FCC_A1,NI:VA;0) = +633
      BMAGN(FCC_A1,NI:VA;0) = +.52
      TC(FCC_A1,AL,NI:VA;0) = -1112
      TC(FCC_A1,AL,NI:VA;1) = +1745
      L(FCC_A1,AL,NI:VA;0) = +AL3NI+1.5*AL2NI2+ALNI3+1.5*RALNI+4*LOALNI
      L(FCC_A1,AL,NI:VA;1) = +2*AL3NI-2*ALNI3
      L(FCC_A1,AL,NI:VA;2) = +AL3NI-1.5*AL2NI2+ALNI3-1.5*RALNI

 ORD_FCC
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
$ This phase has option F set
  5 SUBLATTICES, SITES  .25:  .25:  .25:  .25:  1
    CONSTITUENTS: AL,NI : AL,NI : AL,NI : AL,NI : VA

      G(ORD_FCC,AL:AL:AL:AL:VA;0) = 0.0
      G(ORD_FCC,AL:AL:AL:NI:VA;0) = +AL3NI
      G(ORD_FCC,AL:AL:NI:NI:VA;0) = +AL2NI2
      G(ORD_FCC,AL:NI:NI:NI:VA;0) = +ALNI3
      G(ORD_FCC,AL:NI:NI:NI:VA;0) = 0.0
      L(ORD_FCC,AL,NI:AL,NI:*:*:VA;0) = +RALNI
      L(ORD_FCC,AL,NI:*:*:*:VA;0) = +LOALNI
```

```
Phase: ORD_FCC                , Status:      130  FD
  Subl:  5    0.250    0.250    0.250    0.250    1.000
  Constituents: AL NI: AL NI: AL NI: AL NI: VA:
  + Magnetic model by Inden, anti-ferromagntic factor: -3
    Magnetic function below the ordering temperature TC with TAO=T/TC:
    1-0.860338755*TAO**(-1)-0.17449124*TAO**3-.00775516624*TAO**9
        -.0017449124*TAO**15
    Magnetic function above the ordering temperature TC with TAO=T/TC:
    -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)-.000284601512*TAO**(-25)
  G(ORD_FCC,AL:AL:AL:NI:VA;0)= 298.15 +AL3NI; 6000 N N 03SUN
  G(ORD_FCC,AL:AL:NI:NI:VA;0)= 298.15 +AL2NI2; 6000 N N 03SUN
  G(ORD_FCC,AL:NI:NI:NI:VA;0)= 298.15 +ALNI3; 6000 N N 03SUN
    G(ORD_FCC,*:*:AL,NI:AL,NI:VA;0)= 298.15 +RALNI; 6000 N 03SUN
    G(ORD_FCC,*:*:*:AL,NI:VA;0)= 298.15 +LOALNI; 6000 N N 03SUN
Disordered fraction set parameters, factor:     1.0000  ----------
  GD(ORD_FCC,AL:VA;0)-H298(SER,AL) = 298.15 +GHSERAL; 6000 N 91DIN
  GD(ORD_FCC,NI:VA;0)-H298(SER,NI) = 298.15 +GHSERNI; 6000 N 91DIN
  TCD(ORD_FCC,NI:VA;0)= 298.15 +633; 6000 N 89DIN
  BMAGD(ORD_FCC,NI:VA;0)= 298.15 +0.52; 6000 N 89DIN
    TCD(ORD_FCC,AL,NI:VA;0)= 298.15 -1112; 6000 N 95DUP
    TCD(ORD_FCC,AL,NI:VA;1)= 298.15 +1745; 6000 N 95DUP
    GD(ORD_FCC,AL,NI:VA;0)= 298.15 +AL3NI+1.5*AL2NI2+ALNI3+1.5*RALNI+4*LOALNI; 6000 N 03SUN
    GD(ORD_FCC,AL,NI:VA;1)= 298.15 +2*AL3NI-2*ALNI3; 6000 N 03SUN
    GD(ORD_FCC,AL,NI:VA;2)= 298.15 +AL3NI-1.5*AL2NI2+ALNI3-1.5*RALNI; 6000 N 03SUN
```

The F option allows to handle only one of the configurations that are equivalent by symmetry.

F-4SL Split in 2 (NEVER)

B. Sundman, N. Dupin, JEEP 2003, Lyon

$$G = nG^{dis}(x_i) + \Delta G^{ord}(y_i^s)$$

```
 FCC_A1
$ THIS PHASE IS THE DISORDERED PART OF ORD_FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
 ADDITIONAL CONTRIBUTION FROM MAGNETIC ORDERING
      Magnetic function below Curie Temperature
      +1-.860338755*TAO**(-1)-.17449124*TAO**3-.00775516624*TAO**9
      -.0017449124*TAO**15
      Magnetic function above Curie Temperature
       -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)
      -2.84601512E-04*TAO**(-25)
    CONSTITUENTS: AL,NI

      G(FCC_A1,AL;0)-H298(FCC_A1,AL;0) = +GHSERAL
      G(FCC_A1,NI;0)-H298(FCC_A1,NI;0) = +GHSERNI
      TC(FCC_A1,NI;0) = +633
      BMAGN(FCC_A1,NI;0) = +.52
      TC(FCC_A1,AL,NI;0) = -1112
      TC(FCC_A1,AL,NI;1) = +1745

 ORD_FCC
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
$ This phase has option F set
  4 SUBLATTICES, SITES  .25:  .25:  .25:  .25
    CONSTITUENTS: AL,NI : AL,NI : AL,NI : AL,NI

      G(ORD_FCC,AL:AL:AL:AL:VA;0) = 0.0
      G(ORD_FCC,AL:AL:AL:NI:VA;0) = +AL3NI
      G(ORD_FCC,AL:AL:NI:NI:VA;0) = +AL2NI2
      G(ORD_FCC,AL:NI:NI:NI:VA;0) = +ALNI3
      G(ORD_FCC,AL:NI:NI:NI:VA;0) = 0.0
      L(ORD_FCC,AL,NI:AL:NI:*:*;0) = +RALNI
      L(ORD_FCC,AL,NI:*:*:*;0) = +LOALNI
```

```
Phase: ORD_FCC                , Status:      130  FD
  Subl:  4    0.250    0.250    0.250    0.250
  Constituents: AL NI: AL NI: AL NI: AL NI:
  + Magnetic model by Inden, anti-ferromagntic factor: -3
    Magnetic function below the ordering temperature TC with TAO=T/TC:
    1-0.860338755*TAO**(-1)-0.17449124*TAO**3-.00775516624*TAO**9
        -.0017449124*TAO**15
    Magnetic function above the ordering temperature TC with TAO=T/TC:
    -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)-.000284601512*TAO**(-25)
  G(ORD_FCC,AL:AL:AL:NI;0)= 298.15 +AL3NI; 6000 N N 03SUN
  G(ORD_FCC,AL:AL:NI:NI;0)= 298.15 +AL2NI2; 6000 N N 03SUN
  G(ORD_FCC,AL:NI:NI:NI;0)= 298.15 +ALNI3; 6000 N N 03SUN
    G(ORD_FCC,*:*:AL,NI:AL,NI;0)= 298.15 +RALNI; 6000 N 03SUN
    G(ORD_FCC,*:*:*:AL,NI;0)= 298.15 +LOALNI; 6000 N N 03SUN
Disordered fraction set parameters, factor:     1.0000  ----------
  GD(ORD_FCC,AL;0)-H298(SER,AL) = 298.15 +GHSERAL; 6000 N 91DIN
  GD(ORD_FCC,NI;0)-H298(SER,NI) = 298.15 +GHSERNI; 6000 N 91DIN
  TCD(ORD_FCC,NI;0)= 298.15 +633; 6000 N 89DIN
  BMAGD(ORD_FCC,NI;0)= 298.15 +0.52; 6000 N 89DIN
    TCD(ORD_FCC,AL,NI;0)= 298.15 -1112; 6000 N 95DUP
    TCD(ORD_FCC,AL,NI;1)= 298.15 +1745; 6000 N 95DUP
```

When $\Delta G^{dis}(x_i) = \Delta G^{ord}(y_i^s = x_i)$ in the split in 3, the interaction parameters in the disordered part disappear of the split in 2. The split in 2 term implementation introduced after Ringberg meeting proposition is available in TC or OC softwares under the NEVER option as it has initially introduced for phases that never disorder like the σ phase.

Wild F-4SL

$$G = G^{ord}(y_i^s)$$

B. Sundman, N. Dupin, JEEP 2003, Lyon

```
ORD_FCC
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
ADDITIONAL CONTRIBUTION FROM MAGNETIC ORDERING
     Magnetic function below Curie Temperature
     +1-.860338755*TAO**(-1)-.17449124*TAO**3-.00775516624*TAO**9
     -.0017449124*TAO**15
     Magnetic function above Curie Temperature
      -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)
     -2.84601512E-04*TAO**(-25)
$ This phase has option F set
 4 SUBLATTICES, SITES  .25:  .25:  .25:  .25
   CONSTITUENTS: AL,NI : AL,NI : AL,NI : AL,NI

   G(ORD_FCC,AL:AL:AL:AL;0)-0.75 H298(FCC_A1,AL;0)-0.25 H298(FCC_A1,NI;0) = 0.0
   G(ORD_FCC,AL:AL:AL:NI;0)-0.75 H298(FCC_A1,AL;0)-0.25 H298(FCC_A1,NI;0) = +AL3NI
   G(ORD_FCC,AL:AL:NI:NI;0)-0.5 H298(FCC_A1,AL;0)-0.5 H298(FCC_A1,NI;0) =  +AL2NI2
   G(ORD_FCC,AL:NI:NI:NI;0)-0.25 H298(FCC_A1,AL;0)-0.75 H298(FCC_A1,NI;0) = +ALNI3
   G(ORD_FCC,NI:NI:NI:NI;0)-0.25 H298(FCC_A1,AL;0)-0.75 H298(FCC_A1,NI;0) = 0.0
   G(ORD_FCC,AL:*:*:*;0) = +.25*GHSERAL
   G(ORD_FCC,NI:*:*:*;0) = +.25*GHSERNI
   TC(ORD_FCC,NI:*:*:*;0) = +.25*TCNI
   BMAGN(ORD_FCC,NI:*:*:*;0) = +.25*BMNI
   TC(ORD_FCC,AL,NI:*:*:*;0) = +.25*TCALNI0
   TC(ORD_FCC,AL,NI:*:*:*;1) = +.25*TCALNI1
   L(ORD_FCC,AL,NI:*:*:*;0) = +LOALNI
   L(ORD_FCC,AL,NI:AL,NI:*:*;0) = +RALNI
```

```
Phase: ORD_FCC                , Status:       30  F
 Subl:  4   0.250   0.250   0.250   0.250
 Constituents: AL NI: AL NI: AL NI: AL NI:
 + Magnetic model by Inden, anti-ferromagntic factor: -3
   Magnetic function below the ordering temperature TC with TAO=T/TC:
   1-0.860338755*TAO**(-1)-0.17449124*TAO**3-.00775516624*TAO**9
       -.0017449124*TAO**15
   Magnetic function above the ordering temperature TC with TAO=T/TC:
   -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)-.000284601512*TAO**(-25)

 G(ORD_FCC,AL:AL:AL:NI;0)-0.75*H298(SER,AL)-0.25*H298(SER,NI) = 298.15 +AL3NI
 G(ORD_FCC,AL:AL:NI:NI;0)-0.5*H298(SER,AL)-0.5*H298(SER,NI) = 298.15 +AL2NI2;
 G(ORD_FCC,AL:NI:NI:NI;0)-0.25*H298(SER,AL)-0.75*H298(SER,NI) = 298.15 +ALNI3
 G(ORD_FCC,*:*:*:AL;0)-0.25*H298(SER,AL) = 298.15 +0.25*GHSERAL; 6000 N 91DIN
 G(ORD_FCC,*:*:*:NI;0)-0.25*H298(SER,NI) = 298.15 +0.25*GHSERNI; 6000 N 91DIN
 TC(ORD_FCC,*:*:*:NI;0)= 298.15 +0.25*TCNI; 6000 N 89DIN
 BMAG(ORD_FCC,*:*:*:NI;0)= 298.15 +0.25*BMNI; 6000 N 89DIN
   G(ORD_FCC,*:*:AL,NI:AL,NI:0)= 298.15 +RALNI; 6000 N 03SUN
   TC(ORD_FCC,*:*:*:AL,NI;0)= 298.15 +0.25*TCALNI0; 6000 N 95DUP
   TC(ORD_FCC,*:*:*:AL,NI;1)= 298.15 +0.25*TCALNI1; 6000 N 95DUP
   G(ORD_FCC,*:*:*:AL,NI;0)= 298.15 +LOALNI; 6000 N N 03SUN
```

When all interaction parameters are taken into account in the ordered part, the split is not any more needed using $G(\varphi, i:*:*:*:*;0)$ parameters to take into account the lattice stabilities.

Wild F-4SL using BE

B. Sundman, N. Dupin, JEEP 2003, Lyon

$$G = G^{ord}(y_i^s)$$

```
 ORD_FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
 ADDITIONAL CONTRIBUTION FROM MAGNETIC ORDERING
      Magnetic function below Curie Temperature
      +1-.860338755*TAO**(-1)-.17449124*TAO**3-.00775516624*TAO**9
      -.0017449124*TAO**15
      Magnetic function above Curie Temperature
       -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)
      -2.84601512E-04*TAO**(-25)
$ This phase has option F set
  4 SUBLATTICES, SITES  .25:  .25:  .25:  .25
    CONSTITUENTS: AL,NI : AL,NI : AL,NI : AL,NI

      G(ORD_FCC,AL:AL:AL:AL;0)-0.75 H298(FCC_A1,AL;0)-0.25 H298(FCC_A1,NI;0) = 0.0
      G(ORD_FCC,AL:AL:AL:NI;0)-0.75 H298(FCC_A1,AL;0)-0.25 H298(FCC_A1,NI;0) = +DGAL3NI
      G(ORD_FCC,AL:AL:NI:NI;0)-0.5 H298(FCC_A1,AL;0)-0.5 H298(FCC_A1,NI;0) =  +DGAL2NI2
      G(ORD_FCC,AL:NI:NI:NI;0)-0.25 H298(FCC_A1,AL;0)-0.75 H298(FCC_A1,NI;0) = 0.0
      G(ORD_FCC,NI:NI:NI:NI;0)-0.25 H298(FCC_A1,AL;0)-0.75 H298(FCC_A1,NI;0) = 0.0
      G(ORD_FCC,AL:*:*:*;0) = +.25*GHSERAL
      G(ORD_FCC,NI:*:*:*;0) = +.25*GHSERNI
      TC(ORD_FCC,NI:*:*:*;0) = +.25*TCNI
      BMAGN(ORD_FCC,NI:*:*:*;0) = +.25*BMNI
      G(ORD_FCC,AL:NI:*:*;0) = +UALNI3
      TC(ORD_FCC,AL,NI:*:*:*;0) = +.25*TCALNI0
      TC(ORD_FCC,AL,NI:*:*:*;1) = +.25*TCALNI1
      L(ORD_FCC,AL,NI:*:*:*;0) = +LOALNI
      L(ORD_FCC,AL,NI:AL,NI:*:*;0) = +RALNI

FUNCTION   UALNI3    =  ATHIRD*ALNI3
FUNCTION   DGAL2NI2  =  AL2NI2-4*UALNI3
FUNCTION   DGALNI3   =  AL3NI-3*UALNI3
```

```
Phase: ORD_FCC                , Status:       30  F
 Subl:  4    0.250   0.250   0.250   0.250
 Constituents: AL NI: AL NI: AL NI: AL NI:
 + Magnetic model by Inden, anti-ferromagntic factor: -3
   Magnetic function below the ordering temperature TC with TAO=T/TC:
   1-0.860338755*TAO**(-1)-0.17449124*TAO**3-.00775516624*TAO**9
       -.0017449124*TAO**15
   Magnetic function above the ordering temperature TC with TAO=T/TC:
   -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)-.000284601512*TAO**(-25)

 G(ORD_FCC,AL:AL:AL:NI;0)-0.75*H298(SER,AL)-0.25*H298(SER,NI) = 298.15 +DGAL3
 G(ORD_FCC,AL:AL:NI:NI;0)-0.5*H298(SER,AL)-0.5*H298(SER,NI) = 298.15 +DGAL2NI
 G(ORD_FCC,*:*:AL:NI;0)-0.25*H298(SER,AL)-0.75*H298(SER,NI) = 298.15 +UALNI3;
 G(ORD_FCC,*:*:*:AL;0)-0.25*H298(SER,AL) = 298.15 +0.25*GHSERAL; 6000 N
 G(ORD_FCC,*:*:*:NI;0)-0.25*H298(SER,NI) = 298.15 +0.25*GHSERNI; 6000 N
 TC(ORD_FCC,*:*:*:NI;0)= 298.15 +0.25*TCNI; 6000 N 89DIN
 BMAG(ORD_FCC,*:*:*:NI;0)= 298.15 +0.25*BMNI; 6000 N 89DIN
   G(ORD_FCC,*:*:AL,NI:AL,NI;0)= 298.15 +RALNI; 6000 N 03SUN
   TC(ORD_FCC,*:*:*:AL,NI;0)= 298.15 +0.25*TCALNI0; 6000 N 95DUP
   TC(ORD_FCC,*:*:*:AL,NI;1)= 298.15 +0.25*TCALNI1; 6000 N 95DUP
   G(ORD_FCC,*:*:*:AL,NI;0)= 298.15 +LOALNI; 6000 N N 03SUN
```

Bond energies between pairs are useful to extrapolate more easily into multicomponent databases.
https://doi.org/10.6028/jres.123.020

Wild F-4SL using BE

$$G = G^{ord}(y_i^s)$$

B. Sundman, N. Dupin, JEEP 2003, Lyon

```
 ORD_FCC
 EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
 ADDITIONAL CONTRIBUTION FROM MAGNETIC ORDERING
      Magnetic function below Curie Temperature
      +1-.860338755*TAO**(-1)-.17449124*TAO**3-.00775516624*TAO**9
      -.0017449124*TAO**15
      Magnetic function above Curie Temperature
       -.0426902268*TAO**(-5)-.0013552453*TAO**(-15)
      -2.84601512E-04*TAO**(-25)
$ This phase has option F set
  4 SUBLATTICES, SITES  .25:  .25:  .25:  .25
    CONSTITUENTS: AL,NI : AL,NI : AL,NI : AL,NI

      G(ORD_FCC,AL:AL:AL:AL;0)-0.75 H298(FCC_A1,AL;0)-0.25 H298(FCC_A1,NI;0) = 0.0
      G(ORD_FCC,AL:AL:AL:NI;0)-0.75 H298(FCC_A1,AL;0)-0.25 H298(FCC_A1,NI;0) = +DGAL3NI
      G(ORD_FCC,AL:AL:NI:NI;0)-0.5 H298(FCC_A1,AL;0)-0.5 H298(FCC_A1,NI;0) =  +DGAL2NI2
      G(ORD_FCC,AL:NI:NI:NI;0)-0.25 H298(FCC_A1,AL;0)-0.75 H298(FCC_A1,NI;0) = 0.0
      G(ORD_FCC,NI:NI:NI:NI;0)-0.25 H298(FCC_A1,AL;0)-0.75 H298(FCC_A1,NI;0) = 0.0
      G(ORD_FCC,AL:*:*:*;0) = +.25*GHSERAL
      G(ORD_FCC,NI:*:*:*;0) = +.25*GHSERNI
      TC(ORD_FCC,NI:*:*:*;0) = +.25*TCNI
      BMAGN(ORD_FCC,NI:*:*:*;0) = +.25*BMNI
      G(ORD_FCC,AL:NI:*:*;0) = +UALNI3
      TC(ORD_FCC,AL,NI:*:*:*;0) = +.25*TCALNI0
      TC(ORD_FCC,AL,NI:*:*:*;1) = +.25*TCALNI1
      L(ORD_FCC,AL,NI:*:*:*;0) = +LOALNI
      L(ORD_FCC,AL,NI:AL,NI:*:*;0) = +RALNI
```

$$\left(y_{Al}^{\alpha}y_{Al}^{\beta}y_{Al}^{\gamma}y_{Ni}^{\delta} + y_{Al}^{\alpha}y_{Al}^{\beta}y_{Ni}^{\gamma}y_{Al}^{\delta} + y_{Al}^{\alpha}y_{Ni}^{\beta}y_{Al}^{\gamma}y_{Al}^{\delta} + y_{Ni}^{\alpha}y_{Al}^{\beta}y_{Al}^{\gamma}y_{Al}^{\delta}\right)$$

$$\left(y_{Al}^{\alpha}y_{Al}^{\beta}y_{Ni}^{\gamma}y_{Ni}^{\delta} + y_{Al}^{\alpha}y_{Ni}^{\beta}y_{Al}^{\gamma}y_{Ni}^{\delta} + y_{Ni}^{\alpha}y_{Al}^{\beta}y_{Al}^{\gamma}y_{Ni}^{\delta} + y_{Al}^{\alpha}y_{Ni}^{\beta}y_{Ni}^{\gamma}y_{Al}^{\delta} + y_{Ni}^{\alpha}y_{Al}^{\beta}y_{Ni}^{\gamma}y_{Al}^{\delta} + y_{Ni}^{\alpha}y_{Ni}^{\beta}y_{Al}^{\gamma}y_{Al}^{\delta}\right)$$

$$\left(y_{Al}^{\alpha} + y_{Al}^{\beta} + y_{Al}^{\gamma} + y_{Al}^{\delta}\right)$$

$$\left(y_{Al}^{\alpha}y_{Ni}^{\beta} + y_{Al}^{\alpha}y_{Al}^{\gamma} + y_{Al}^{\alpha}y_{Ni}^{\delta} + y_{Al}^{\beta}y_{Al}^{\gamma} + y_{Al}^{\beta}y_{Ni}^{\delta} + y_{Al}^{\gamma}y_{Ni}^{\delta} + y_{Ni}^{\alpha}y_{Al}^{\beta} + y_{Ni}^{\alpha}y_{Al}^{\gamma} + y_{Ni}^{\alpha}y_{Al}^{\delta} + y_{Ni}^{\beta}y_{Al}^{\gamma} + y_{Ni}^{\beta}y_{Al}^{\delta} + y_{Ni}^{\gamma}y_{Al}^{\delta}\right)$$

$$\left(y_{Al}^{\alpha}y_{Ni}^{\beta} + y_{Al}^{\beta}y_{Ni}^{\beta} + y_{Al}^{\gamma}y_{Ni}^{\gamma} + y_{Al}^{\delta}y_{Ni}^{\delta}\right)$$

$$\left(y_{Al}^{\alpha}y_{Ni}^{\alpha}y_{Al}^{\beta}y_{Ni}^{\beta} + y_{Al}^{\alpha}y_{Ni}^{\alpha}y_{Al}^{\gamma}y_{Ni}^{\gamma} + y_{Al}^{\alpha}y_{Ni}^{\alpha}y_{Al}^{\delta}y_{Ni}^{\delta} + y_{Al}^{\beta}y_{Ni}^{\beta}y_{Al}^{\gamma}y_{Ni}^{\gamma} + y_{Al}^{\beta}y_{Ni}^{\beta}y_{Al}^{\delta}y_{Ni}^{\delta} + y_{Al}^{\gamma}y_{Ni}^{\gamma}y_{Al}^{\delta}y_{Ni}^{\delta}\right)$$

Recommendations

- F-4SL

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- ⇝ F-4SL
- ⇝ Avoid independent assessment of the disordered state

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- ⇝ F-4SL
- ⇝ Avoid independent assessment of the disordered state
- ⇝ Forget 3 terms split.

$$G_{\mathrm{m}} = G_{\mathrm{m}}^{\mathrm{dis}}(x_i) + G_{\mathrm{m}}^{\mathrm{ord}}(y_i', y_i'') - G_{\mathrm{m}}^{\mathrm{ord}}(x_i)$$

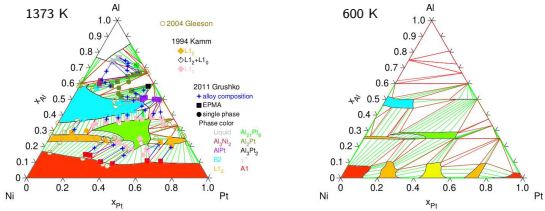
I. Ansara, N. Dupin, H.L. Lukas, B. Sundman,
Journal of Alloys and Compounds, 247 20-30 (1997)

Recommendations

- F-4SL
- Avoid independent assessment of the disordered state
- Forget 3 terms split.
- Explore wild 4SL using BEF

Thank you

4SL : N. Dupin, C. Desgranges, E. Menou, SafranTech CF193687, 2019
A1, $L1_2$, $L1_0$ and $L6_0$: $(Al,Ni,Pt)_{0.25}(Al,Ni,Pt)_{0.25}(Al,Ni,Pt)_{0.25}(Al,Ni,Pt)_{0.25}$



L12-2SL=4SL : Xuan L. Liu *et al.*, Calphad 55 (2016) 88-102
A1 and $L1_2$: $(Al,Ni,Pt)_{0.75}(Al,Ni,Pt)_{0.25}$, $L1_0$ and $L6_0$: $(Al,Ni,Pt)_{0.25}(Al,Ni,Pt)_{0.25}(Ni,Pt)_{0.5}$

