Report of OpenCalphad Calculation

2021-08-22

Materials

Element	CR	NI	FE
Mole-frac	0.25	0.07	0.68

Database

SAF2507.TDB

Equilibrium calculations

Equilibrium 1:

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM 2021.08.22

Conditions :

```
 1:T=1000, 2:P=100000, 3:N=1, 4:X(CR)=0.44533, 5:X(NI)=.02427
 Degrees of freedom are 0
```

Some global data, reference state SER :

```
 T= 1000.00 K ( 726.85 C), P= 1.0000E+05 Pa, V= 3.4138E-06 m3
 N= 1.0000E+00 moles, B= 5.4201E+01 g, RT= 8.3145E+03 J/mol
 G= -4.35107E+04 J, G/N=-4.3511E+04 J/mol, H= 2.8048E+04 J, S= 7.156E+01 J/K
```

Some data for components :

```
  Component name   Moles        Mass-fr   Chem.pot/RT   Activities   Ref.state
  CR               4.4533E-01   0.42721   -4.8628E+00   7.7289E-03   SER (default)
  FE               5.3040E-01   0.54651   -5.3871E+00   4.5754E-03   SER (default)
  NI               2.4270E-02   0.02628   -8.6638E+00   1.7273E-04   SER (default)
```

Some data for phases :

```
  Name             Status  Mass         Volume     Form.Units    Cmp/FU    dGm/RT     Comp:
  SIGMA            E       5.420E-02    3.41E-06   3.33E-02      30.00     0.00E+00   W:
    FE  5.46507E-01   CR  4.27213E-01   NI  2.62801E-02
```

Equilibrium 2:

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM 2021.08.22

Conditions :

```
 1:T=1200, 2:P=100000, 3:N=1, 4:X(CR)=0.4, 5:X(NI)=0.4
 Degrees of freedom are 0
```

Some global data, reference state SER :

```
 T= 1200.00 K ( 926.85 C), P= 1.0000E+05 Pa, V= 4.4348E-06 m3
 N= 1.0000E+00 moles, B= 5.5444E+01 g, RT= 9.9774E+03 J/mol
 G= -6.34093E+04 J, G/N=-6.3409E+04 J/mol, H= 3.2362E+04 J, S= 7.981E+01 J/K
```

Some data for components :

```
  Component name   Moles        Mass-fr   Chem.pot/RT   Activities   Ref.state
  CR               4.0000E-01   0.37513   -4.9927E+00   6.7874E-03   SER (default)
  FE               2.0000E-01   0.20145   -7.2673E+00   6.9799E-04   SER (default)
  NI               4.0000E-01   0.42342   -7.2619E+00   7.0180E-04   SER (default)
```

Some data for phases :

```
  Name             Status  Mass         Volume     Form.Units    Cmp/FU    dGm/RT     Comp:
  BCC_A2           E       4.457E-03    5.99E-07   8.45E-02      1.00      0.00E+00   W:
    CR  8.24657E-01   FE  1.24307E-01   NI  5.10365E-02
  FCC_A1#1         E       5.099E-02    3.84E-06   9.16E-01      1.00      0.00E+00   W:
    NI  4.55969E-01   CR  3.35833E-01   FE  2.08198E-01
```

Equilibrium 3:

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM 2021.08.22

Conditions :

```
 1:T=1200, 2:P=100000, 3:N=1, 4:X(CR)=0.4, 5:X(NI)=0.4
 Degrees of freedom are 0
```

Some global data, reference state SER :

```
T= 1200.00 K ( 926.85 C), P= 1.0000E+05 Pa, V= 4.4348E-06 m3
N= 1.0000E+00 moles, B= 5.5444E+01 g, RT= 9.9774E+03 J/mol
G= -6.34093E+04 J, G/N=-6.3409E+04 J/mol, H= 3.2362E+04 J, S= 7.981E+01 J/K
```

Some data for components :

Component name	Moles	Mass-fr	Chem.pot/RT	Activities	Ref.state
CR	4.0000E-01	0.37513	-4.9927E+00	6.7874E-03	SER (default)
FE	2.0000E-01	0.20145	-7.2673E+00	6.9799E-04	SER (default)
NI	4.0000E-01	0.42342	-7.2619E+00	7.0180E-04	SER (default)

Some data for phases :

Name	Status	Mass	Volume	Form.Units	Cmp/FU	dGm/RT	Comp:
BCC_A2	E	4.457E-03	5.99E-07	8.45E-02	1.00	0.00E+00	W:
CR 8.24657E-01	FE 1.24307E-01	NI 5.10365E-02					
FCC_A1#1	E	5.099E-02	3.84E-06	9.16E-01	1.00	0.00E+00	W:
NI 4.55969E-01	CR 3.35833E-01	FE 2.08198E-01					

Phase diagram calculations

Figure 1: Tenary phase diagram

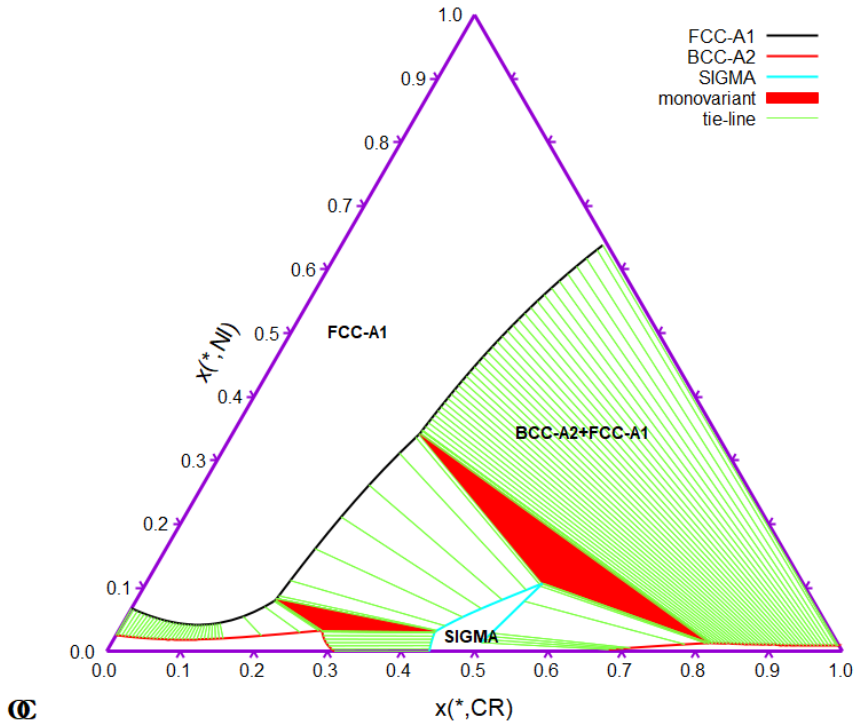

Figure 2: Tenary phase diagram

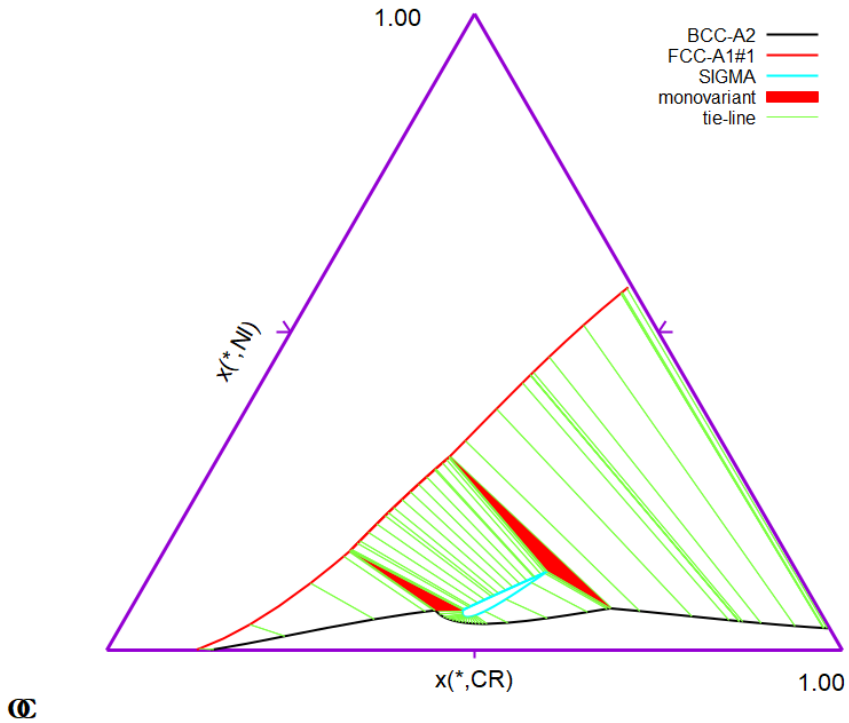

Figure 3: Tenary phase diagram