Report of OpenCalphad Calculation

2021-08-22

Materials

Element	CU	AG
Mole-frac	0.2	0.8

Database

AGCU.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(CU)=0.2
Degrees of freedom are 0
```

Some global data, reference state SER :

```
T= 1000.00 K ( 726.85 C), P= 1.0000E+05 Pa, V= 0.0000E+00 m3
N= 1.0000E+00 moles, B= 9.9005E+01 g, RT= 8.3145E+03 J/mol
G= -5.46597E+04 J, G/N=-5.4660E+04 J/mol, H= 2.1683E+04 J, S= 7.634E+01 J/K
```

Some data for components :

```
Component name   Moles        Mass-fr   Chem.pot/RT   Activities   Ref.state
AG               8.0000E-01   0.87163   -6.8174E+00   1.0945E-03   SER (default)
CU               2.0000E-01   0.12837   -5.6004E+00   3.6964E-03   SER (default)
```

Some data for phases :

```
Name             Status  Mass        Volume     Form.Units    Cmp/FU    dGm/RT     Comp:
FCC_A1#1         E       9.170E-02   0.00E+00   8.88E-01      1.00      0.00E+00   W:
  AG  9.36598E-01   CU  6.34020E-02
FCC_A1_AUTO#2    E       7.303E-03   0.00E+00   1.12E-01      1.00      0.00E+00   W:
  CU  9.44150E-01   AG  5.58503E-02
```

Phase diagram calculations

Figure 1: Binary phase diagram

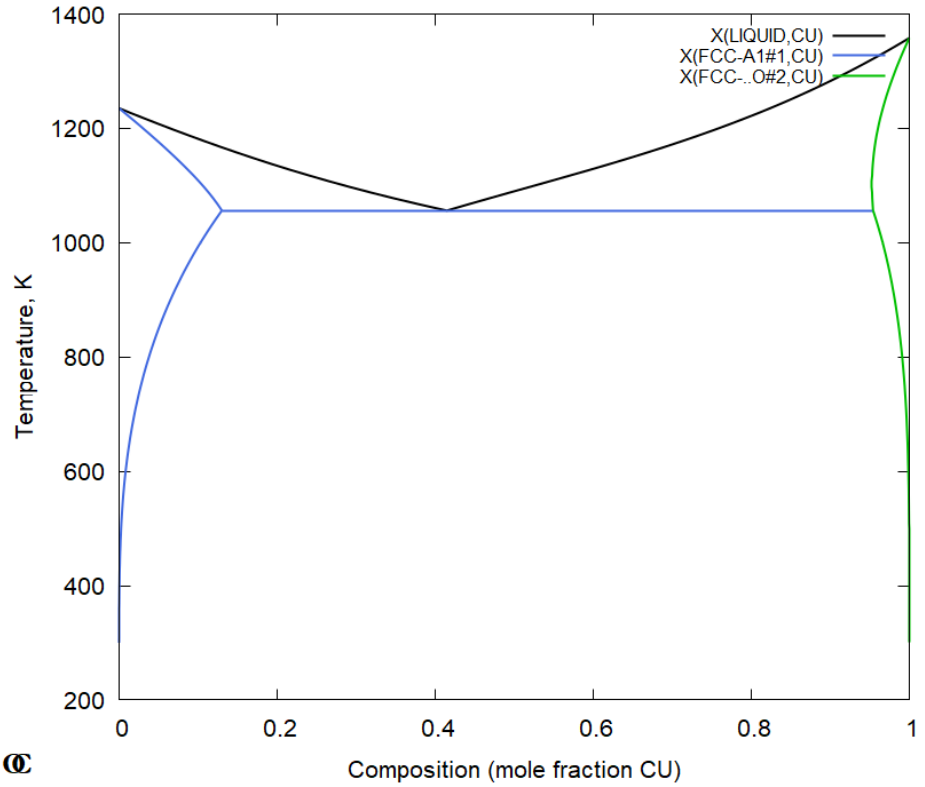

Figure 2: Composition vs. Gibbs energy

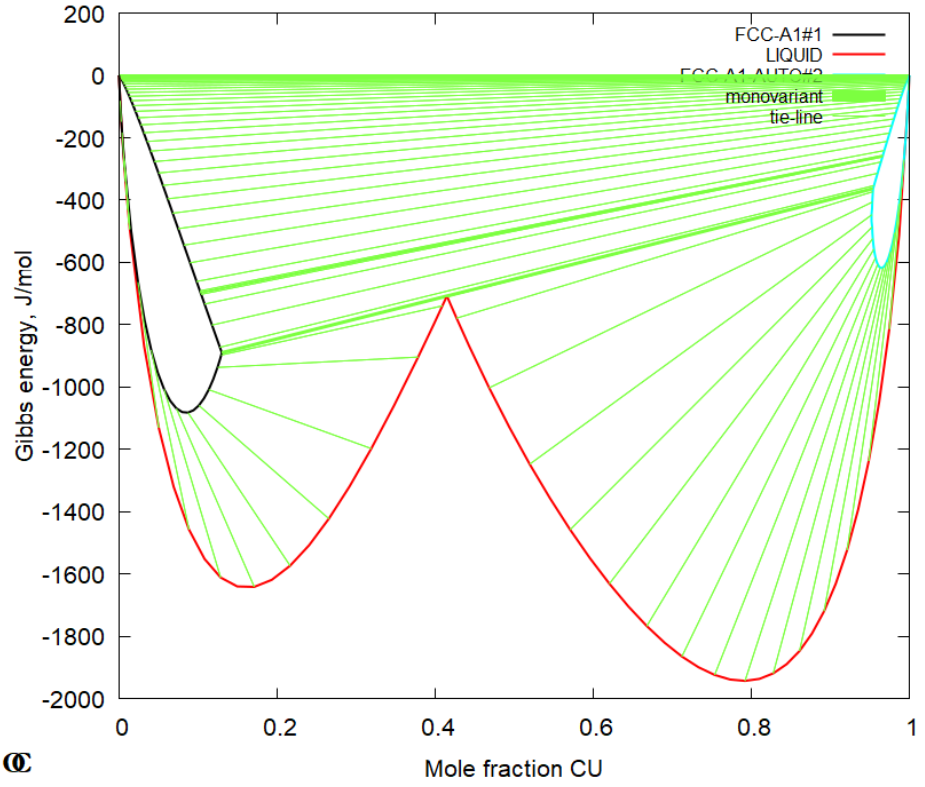

Figure 3: Temperature vs. Activity