OpenCalphad　磁気モデル　　OpenCalphad magnetic　　2026 年 2 月 11 日

Q1　OpenCalphad ソフトウェアは 2001Chen の磁気モデルをサポートしていますか？

A1　はい、サポートしています。

本書は OpenCalphad 6.084 を用います。(2025 年 5 月 13 日版)

Q2　熱力学データベース TDB ファイルの中、どう書けば良いですか？

A2-1　TYPE-DEF 行を

TYPE-DEF A GES AMEND_PHASE_DESCRIPTION FCC MAGNETIC 0.0 0.25 !

TYPE-DEF B GES AMEND_PHASE_DESCRIPTION BCC MAGNETIC 0.0 0.37 !

とします。

出典：　ochelp.pdf

**5.11.2.2　*amend phase ... addition* Magnetic_contrib**

The Inden-Hillert and the modified Inden-Qing-Xiong model for the magnetic contribution to the Gibbs energy can be set by this command This depends on model parameters describing the Curie and Neel temperatures and the Bohr magneton number, as listed in model parameters identifiers 2.8.1, for the phase.

You also must also enter model parameters for the constituents of the phase, see the documentation of the model or Lukas [4].

**Antiferromagnetic factor:**

The Qing-Xiong model is selected by giving zero (0) for the question about the anti-ferromagnetic factor. For the original Inden-Hillert model -3 is used for FCC and HCP whereas -1 is used for BCC.

The Inden-Hillert model is described in Lukas et al [4]. The Inden-Qing-Xiong modified model requires separate values of the Curie and Neel Temperatures and either an "effective" Bohr magneton number or individual Bohr magneton numbers for the constituents of the phase.

A2-2　CTA, NTA, IBM パラメータを書きます。

出典：

- TC, a parameter for the critical temperature for ferro or antiferro magnetic ordering using the Inden model.
- BMAG, a parameter for the average Bohr magneton number using the Inden model.
- CTA, a parameter for the Curie temperature for ferromagnetic ordering using a modified Inden model.
- NTA, a parameter for the Neel temperature for antiferromagnetic ordering using a modified Inden model.
- IBM&C, a parameter for the individual Bohr magneton number for constituent C using a modified Inden model. For example IBM&FE(BCC,FE) is the Bohr magneton number for BCC Fe.

具体的には、

```
PARA    CTA(BCC_A2,FE:VA)          +1043;
PARA    NTA(BCC_A2,FE:VA)          -1043;
PARA    IBM&FE(BCC_A2,FE:VA)       +2.22;
```

```
, FCC_A1    -67;
, FCC_A1    +67;
, FCC_A1    +0.7;
```

Q3　どの磁気モデルがセットされたか、確認できますか？

A3　はい、LIST コマンドを利用し、指定した相の情報を確認できます。

A3-1　従来の磁気モデル　　p=0.4 , D=1.558285 を含む形

```
BCC_A2                        model: CEF-TDB-RKM?
   Number of sublattices:   2, status:          18          0
   + Volume model P*V0(x)*exp(VA(x,T))
   + Magnetic model by Inden, anti-ferromagnetic factor: -1
      Magnetic function below the ordering temperature TC with TAO=T/TC:
      +1-0.905299383*TAO**(-1)-0.153008346*TAO**3-.00680037095*TAO**9
           -.00153008346*TAO**15
      Magnetic function above the ordering temperature TC with TAO=T/TC:
      -.0641731208*TAO**(-5)-.00203724193*TAO**(-15)-.000427820805*TAO**(-25)
   Subl. 1, sites: 1, const.: FE=1
   Subl. 2, sites: 3, const.: VA=1
--->OC6:
```

A3-2　2001Chen の磁気モデル

```
--->OC6: list
phase
Phase name: BCC_A2
model
```

p=0.37 , D=1.180106 を含む形

```
BCC_A2                        model: CEF-TDB-RKM?
   Number of sublattices:   2, status:   4000018          0
   + Volume model P*V0(x)*exp(VA(x,T))
   + Inden magnetic model modified by Qing and Xiong          5
      with separate Curie and Neel temperatures.
      Magnetic function below the ordering temperature TC    with TAO=T/TC:
      +1-0.880323235*TAO**(-1)-0.152870878*TAO**3-.00679426123*TAO**9
           -.00152870878*TAO**15-.000567238878*TAO**21
      Magnetic function above the ordering temperature TC with TAO=T/TC:
      -.0403514888*TAO**(-7)-.00134504963*TAO**(-21)-.000284834039*TAO**(-35)
           -.000102937472*TAO**(-49)
   Subl. 1, sites: 1, const.: FE=1
   Subl. 2, sites: 3, const.: VA=1
--->OC6:
```

Q4　純 Fe 元素に関するギブス自由エネルギー値は？

元素 Fe だけを選択し、温度 1000 ケルビンの平衡計算を行います。

A4-1　従来の磁気モデルで、lattice stability に GHSERFE を用いた場合、

```
--->OC6: list
Output for equilibrium:     1, DEFAULT_EQUILIBRIUM                2026.01.29
Conditions .....................................................:
   1:T=1000, 2:P=100000, 3:N=1
 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=     5.5847E+01 g, RT=     8.3145E+03 J/mol
G= -4.22725E+04 J, G/N=-4.2272E+04 J/mol, H= 2.4689E+04 J, S= 6.696E+01 J/K

Some data for components ....................................:
Component name      Moles          Mole-fr    Chem.pot/RT    Activities    Ref.state
FE                      1.0000E+00    1.00000 -5.0842E+00    6.1940E-03    SER (default)

Some data for phases ......................................:
Name                      Status Moles          Volume       Form.Units Cmp/FU dGm/RT    Comp:
BCC_A2..................... E    1.000E+00    0.00E+00    1.00E+00       1.00    0.00E+00    X:
 FE        1.00000E+00

--->OC6: show G
 G= -4.2272484E+04
```

A4-2　2001Chen モデルで、lattice stability に GHSERFE を用いた場合、

```
--->OC6: list
Output for equilibrium:     1, DEFAULT_EQUILIBRIUM                2026.01.29
   一部略
T=     1000.00 K (     726.85 C), P=    1.0000E+05 Pa, V=    0.0000E+00 m3
N=     1.0000E+00 moles, B=     5.5847E+01 g, RT=     8.3145E+03 J/mol
G= -4.20203E+04 J, G/N=-4.2020E+04 J/mol, H= 2.4986E+04 J, S= 6.701E+01 J/K
   一部略
Name                      Status Moles          Volume       Form.Units Cmp/FU dGm/RT    Comp:
BCC_A2..................... E    1.000E+00    0.00E+00    1.00E+00       1.00    0.00E+00    X:
 FE        1.00000E+00

--->OC6:show G
 G= -4.2020255E+04
```

A4-3　2001Chen モデルで、lattice stability に 3rd generation を用いた場合、

G = +GGBCCL +GMOD(∞) + GEIN + GMAG =

```
--->OC6:list
Output for equilibrium:     1, DEFAULT_EQUILIBRIUM                2026.01.29
Conditions .....................................................:
   1:T=1000, 2:P=100000, 3:N=1
 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=     5.5847E+01 g, RT=     8.3145E+03 J/mol
G= -4.22428E+04 J, G/N=-4.2243E+04 J/mol, H= 2.4607E+04 J, S= 6.685E+01 J/K

Some data for components .....................................:
Component name       Moles          Mole-fr    Chem.pot/RT    Activities    Ref.state
FE                        1.0000E+00    1.00000 -5.0806E+00    6.2161E-03    SER (default)

Some data for phases .....................................:
Name                        Status Moles         Volume       Form.Units Cmp/FU dGm/RT    Comp:
BCC_A2..................... E    1.000E+00    0.00E+00    1.00E+00       1.00    0.00E+00    X:
 FE        1.00000E+00

--->OC6:show G
 G= -4.2242801E+04

--->OC6:show GM(FCC_A1)
 GM(FCC_A1)= -4.1911174E+04
```

次に温度 1200 と 1600 ケルビンでの値を計算してみると、

T = 1200.00 K

```
--->OC6:show GM(BCC_A2)
 GM(BCC_A2)= -5.6602004E+04

--->OC6:show GM(FCC_A1)
 GM(FCC_A1)= -5.6612745E+04
```

T = 1600.00 K

```
--->OC6:show GM(BCC_A2)
 GM(BCC_A2)= -8.9277129E+04

--->OC6:show GM(FCC_A1)
 GM(FCC_A1)= -8.9306647E+04
```

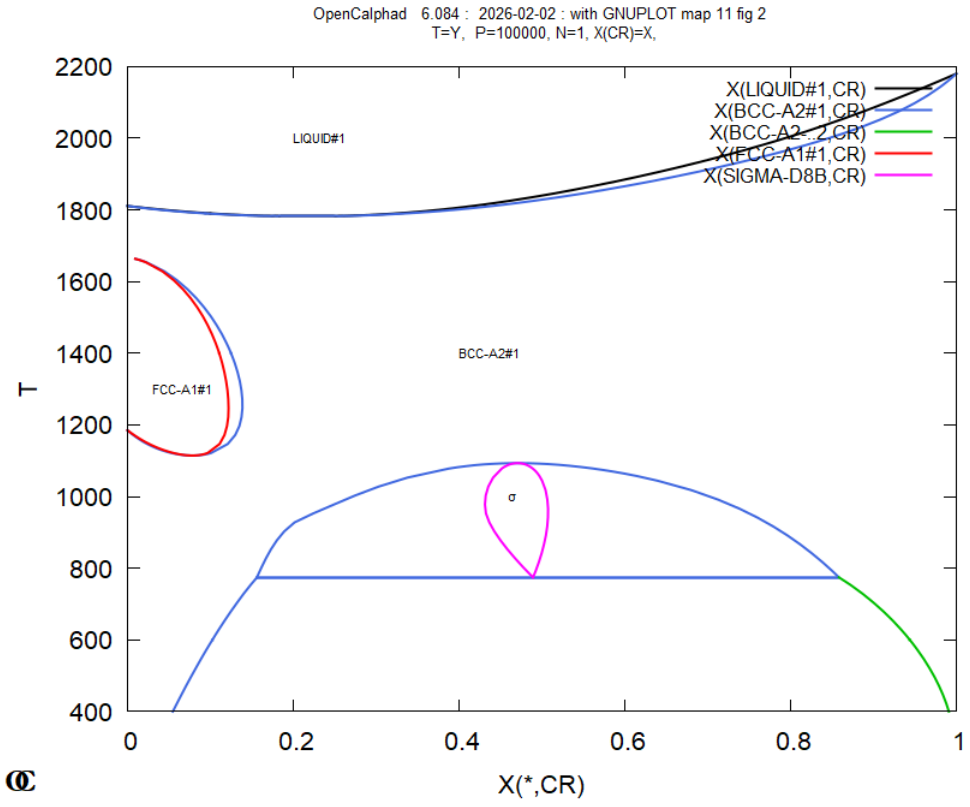
さらに温度 50 ケルビンでの値を計算してみると、

```
T=       50.00 K (   -223.15 C), P=   1.0000E+05 Pa, V=   0.0000E+00 m3
N=     1.0000E+00 moles, B=     5.5847E+01 g, RT=     4.1573E+02 J/mol
G= -4.56718E+03 J, G/N=-4.5672E+03 J/mol, H=-4.5324E+03 J, S= 6.961E-01 J/K
Some data for phases .....:
Name                    Status Moles         Volume      Form.Units Cmp/FU dGm/RT    Comp:
BCC_A2..... E    1.000E+00   0.00E+00   1.00E+00      1.00   0.00E+00   X:

--->OC6:show G
 G= -4.5671812E+03

--->OC6:show GM(FCC_A1)
 GM(FCC_A1)=   1.2577473E+03
```

純 Fe 元素の自由エネルギー値が得られた。

A4-4　OpenCalphad を用いた Fe-Cr 二元系状態図を下に示します。

ベースにした熱力学パラメータは 2011Xio です。
操作コマンドは map11.OCM と同じです。　縦軸・温度の単位はケルビンです。



文献：


2001Chen　Modeling of thermodynamic properties for Bcc, Fcc, Liquid, and Amorphous Iron.
Qing.Chen, Bo.Sundman,
Journal Phase Equilibria, 22 (2001), 631-644.

磁気過剰ギブスエネルギー　$G^{Mag} = R*T*LN(\beta + 1)*g(\tau)$

g($\tau$)は、本書の 2 ページと 7 ページの Magnetic function になる
$\tau < 1$ ： $\tau^{(3)} + \tau^{(9)} + \tau^{(15)} + \tau^{(21)}$
$\tau > 1$ ： $\tau^{(-7)} + \tau^{(-21)} + \tau^{(-35)} + \tau^{(-49)}$

2011Xio　An improved thermodynamic modeling of the Fe-Cr system down to zero kelvin
Copled with key experiments.
W. Xiong, P. Hedstrom, M. Selleby, J. Odqvist, M. Thuvander, Q. Chen,
CALPHAD, 35 (2011), 355-366.

2012Xio　An improved magnetic model for thermodynamic modeling.
Wei Xiong, Q.Chen, P.Korzhavyi, M.Selleby,
CALPHAD, 39 (2012), 11-20.

2014Nar　Thermodynamics of stable and metastable structures in Fe-C system.
R. Naraghi, M. Selleby, J. Agren,
CALPHAD, 46 (2014), 148-158.

2015Abe　TDB ファイル作成で学ぶ　カルファド法による状態図計算.
阿部太一, 内田老鶴圃, (2015).

2022He　A third generation calphad description of Fe : Revisions of Fcc, Hcp and Liquid.
Z.He, F.Haglof, Q.Chen, A.Blomqvist, M.Selleby,
Journal Phase Equilibria, 43 (2022), 287-303.

2024He　Third generation calphad for key elements.
Z.He, Q.Chen, M.Selleby,
Journal Phase Equilibria, 45 (2024), 1163-1181.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## 付録　　FCC 相の磁気モデル情報

従来の磁気モデル　　（p 値=0.28 と D 値=2.342457 を含む形）

```
--->OC6:list
LIST what? /RESULTS/: phase
Phase name:FCC_A1
List what for phase? /CONSTITUTION/: model
For equilibrium:     1, DEFAULT_EQUILIBRIUM
FCC_A1                          model: CEF-TDB-RKM?
  Number of sublattices:   2, status:          18          0
  + Volume model P*V0(x)*exp(VA(x,T))
  + Magnetic model by Inden, anti-ferromagnetic 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)
  Subl. 1, sites: 1, const.: FE=1
  Subl. 2, sites: 1, const.: VA=1
--->OC6:
```

2001Chen の磁気モデル

Antiferromagnetic factor を 0 にした

（p 値=0.25 と D 値=1.82421 を含む形）

```
--->OC6:list
LIST what? /RESULTS/: phase
Phase name:FCC_A1
List what for phase? /CONSTITUTION/: model
For equilibrium:     1, DEFAULT_EQUILIBRIUM
FCC_A1                          model: CEF-TDB-RKM?
  Number of sublattices:   2, status:    4000018          0
  + Volume model P*V0(x)*exp(VA(x,T))
  + Inden magnetic model modified by Qing and Xiong          1
    with separate Curie and Neel temperatures.
    Magnetic function below the ordering temperature TC    with TAO=T/TC:
    +1-0.842849633*TAO**(-1)-0.174242226*TAO**3-.00774409892*TAO**9
        -.00174242226*TAO**15-.000646538871*TAO**21
    Magnetic function above the ordering temperature TC with TAO=T/TC:
    -.0261039233*TAO**(-7)-.000870130777*TAO**(-21)-.000184262988*TAO**(-35)
        -6.65916411E-05*TAO**(-49)
  Subl. 1, sites: 1, const.: FE=1
  Subl. 2, sites: 1, const.: VA=1
--->OC6:
```