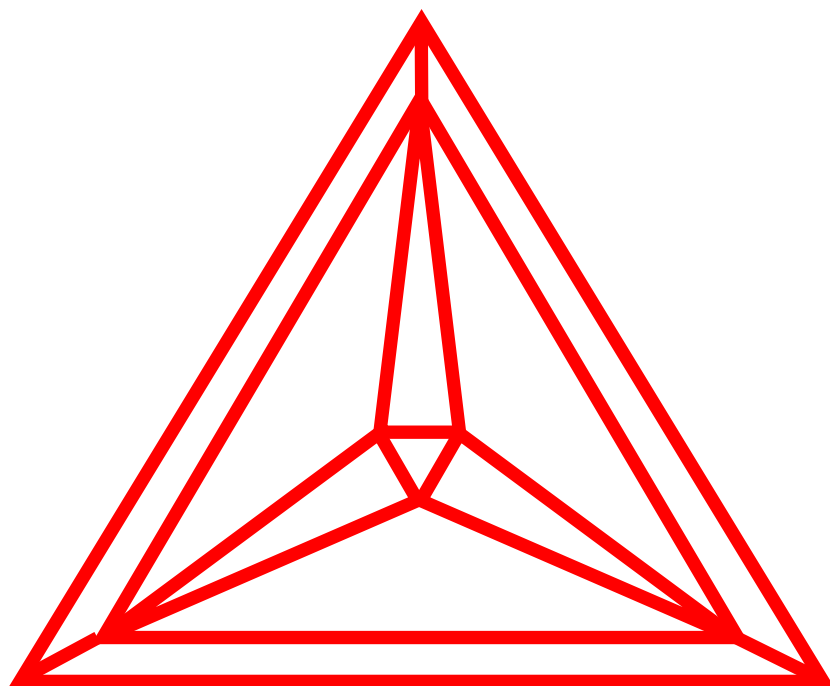


TCWTM

(Thermo-Calc[®] Windows)

Examples Book

Version 5.0



**Thermo-Calc Software AB
Stockholm Technology Park
Björnnäsvägen 21
SE-113 47 Stockholm, Sweden**

Copyright:

The Thermo-Calc® Windows (TCW™) software is the exclusive copyright properties of the Thermo-Calc Software AB (TCS), Stockholm, Sweden. All rights are reserved worldwide!

The TCW™ Users' Guide and TCW™ Examples Book, as well as all other related documentation, are the copyright property of Thermo-Calc Software AB.

It is absolutely forbidden to make any illegal copies of the TCS-provided software, databases, programming interfaces, and their manuals (Users' Guide and Examples Book) and other technical publications (Reference Book and Technical Information). Any unauthorized duplication of such copyrighted products, is a violation of international copyright law. Individuals or organizations (companies, research companies, governmental institutes, and universities) that make or permit to make unauthorized copies may be subject to prosecution.

The utilization of the Thermo-Calc® (TCC™ and TCW™) and DICTRA®™ software and associated database and programming interfaces, as well as their manuals and other technical information, are extensively and permanently governed by the ***Thermo-Calc Software END USER LICENSE AGREEMENT (EULA)***, which is connected with the software.

Disclaimers:

Thermo-Calc Software AB and STT (Foundation of Computational Thermodynamics, Stockholm, Sweden) reserve the rights to further developments of the Thermo-Calc® (TCC™ and TCW™) and DICTRA®™ software and associated database and programming interface products, and to revisions of their manuals and other publications, with no obligation to notify any individual or organization of such developments and revisions. In no event shall Thermo-Calc Software AB and the STT Foundation be liable to any loss of profit or any other commercial damage, including but not limited to special, consequential or other damage.

There may be some minor differences in contents between this Examples Book and the actual appearance of the program as seen on the screen when running the TCW5 (Thermo-Calc Windows version 5). This is because that some of the contents may need to be updated along with the continuous development of the program. Please visit the Thermo-Calc Software web site (www.thermocalc.com) for any patch (with modifications and/or improvements that have been incorporated into the program and its on-line help), or any amendment that have made to the content of the User's Guides and Examples Books, or to the FAQ lists and other technical information publications.


Acknowledgement of Copyright and Trademark Names:

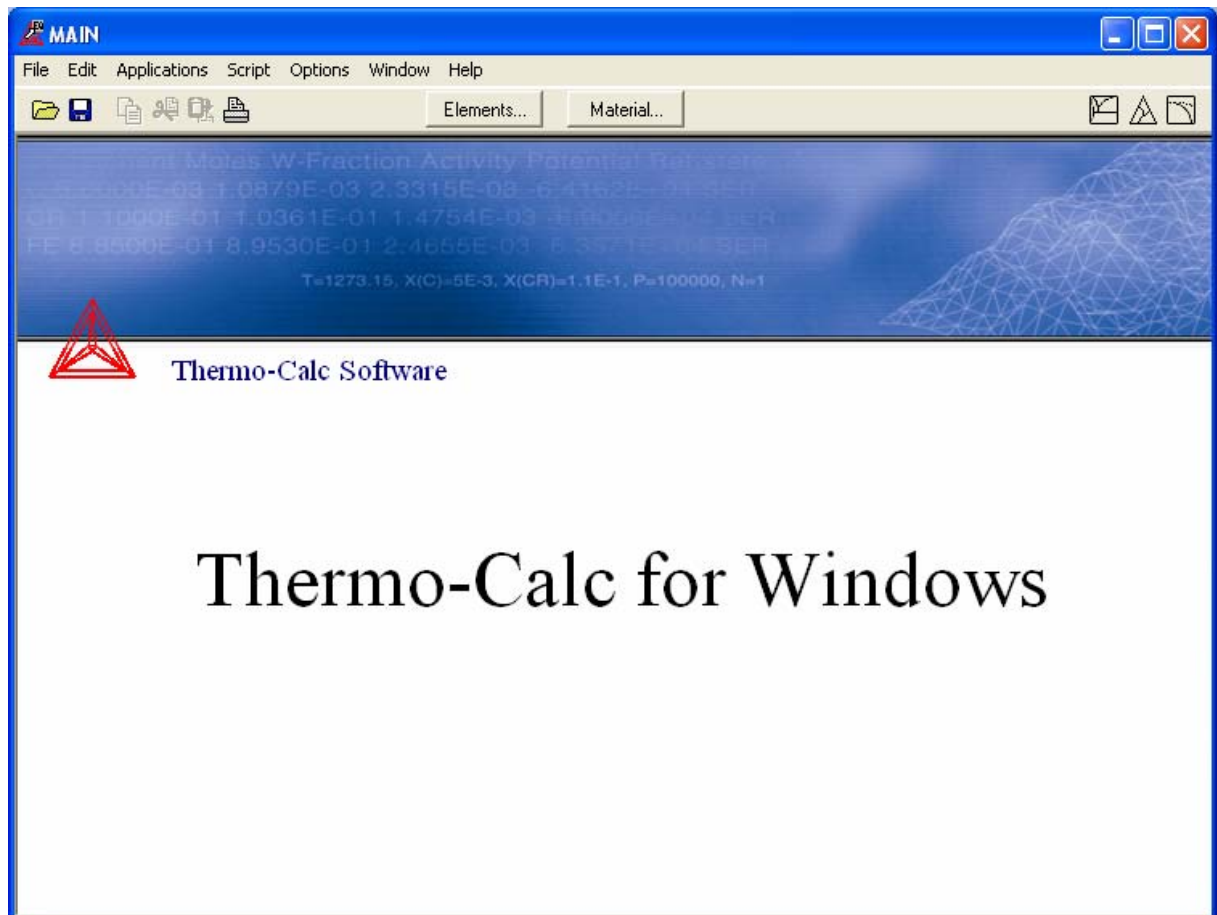
Various names that are protected by copyright and/or trademarks are mentioned for descriptive purposes, within this TCW5 Examples Book and other documents of the Thermo-Calc® (TCC™ and TCW™) and DICTRA®™ software/database/interface packages. Due acknowledgement is herein made of all such protections.

CONTENT

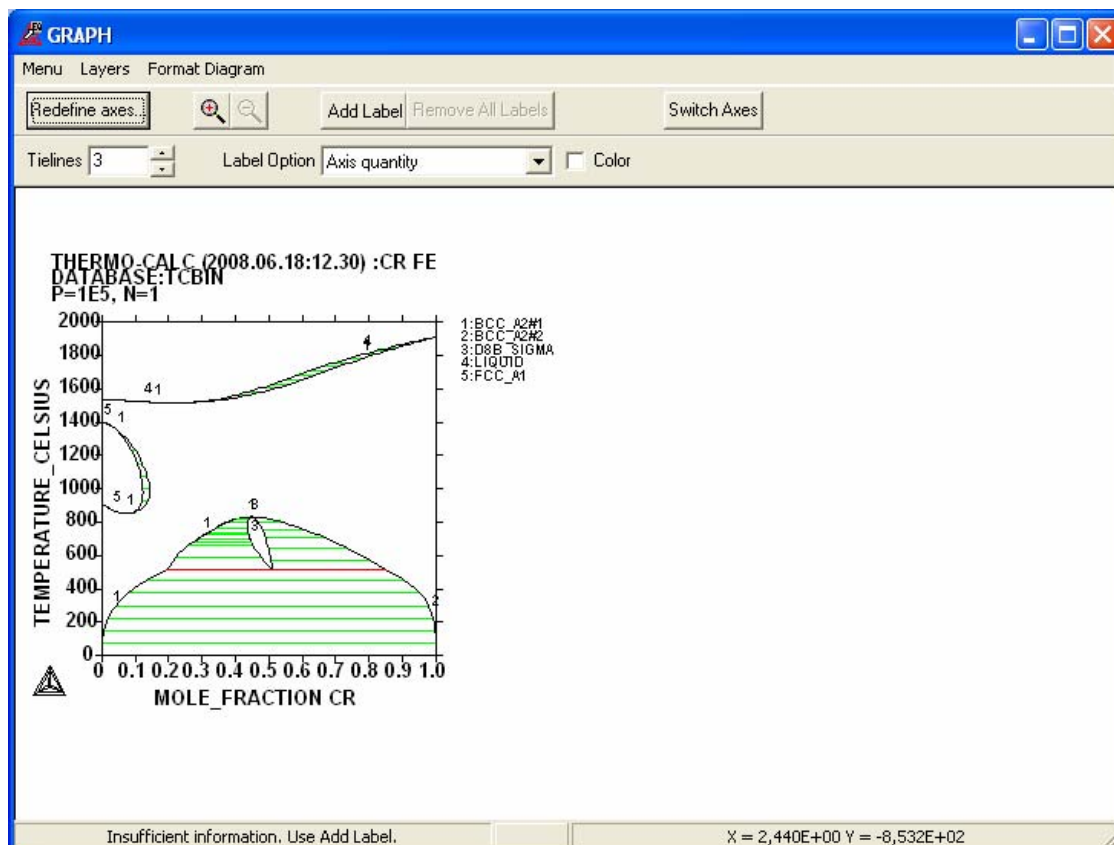
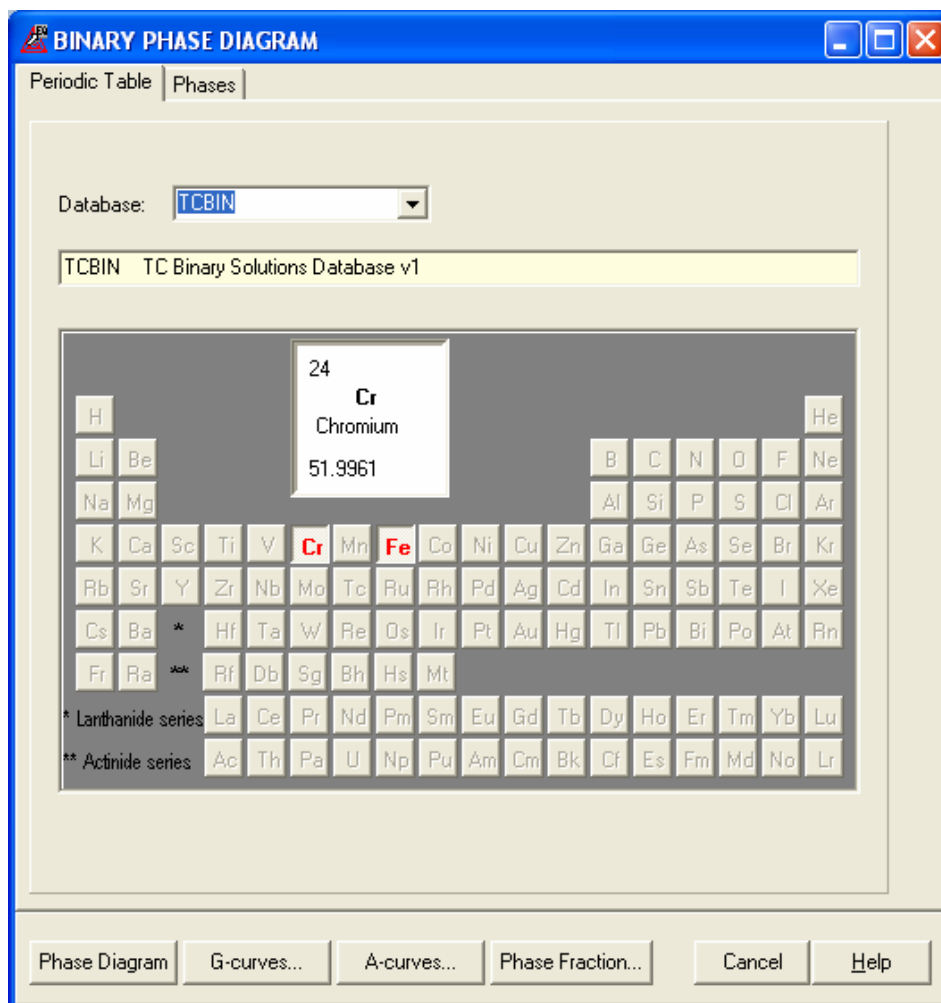
1	Calculation of the Fe-Cr Phase Diagram	4
2	Plotting Thermodynamic Functions	6
3	Calculation of Single Equilibrium in Low Alloyed Fe-Mn-Si-Cr-Ni-C Steel	12
4	Isothermal Section of the Fe-Cr-C System at 1000 K	16
5	Calculation of Isopleth in Fe-8Cr-C System	16
6	Calculation of a Vertical Section for Mixing of Fe-1Cr-0.1C and Fe-20Cr-2C Alloys	24
7	Calculation of Property Diagram of a High Speed Steel	28
8	Calculate Heat and Heat Capacity Variation during Solidification of an Al-Mg-Si Alloy	35
9	Calculate Second Order Transition Line in Al-Fe System	40
10	Calculate CaO-SiO₂ System	51
11	Calculate A₃ Temperature and Its Dependence on Alloying Element	55
12	Mapping of Univariant Equilibria of Liquid in the Fe-C-Cr System	58
13	Plotting of Partial Pressure of Gas Species Along Solubility Lines in As-Ga Phase Diagram	61
14	Scheil-Gulliver Simulation of Solidification for an Al-based Alloy	65
15	Scheil-Gulliver Simulation of Solidification for a Steel with Back Diffusion of Carbon in Solid Phases	69
16	Calculation of Pitting Resistance Equivalence (PRE) for a Duplex Stainless Steel	75
17	Calculation of Speciation of a Gas	85
18	Calculation Using Script and how to Implement a Figure to a Word/PowerPoint file	90

1 Calculation of the Fe-Cr Phase Diagram

1. Open the TCW program by double-clicking its shortcut icon.
2. Click the  button.

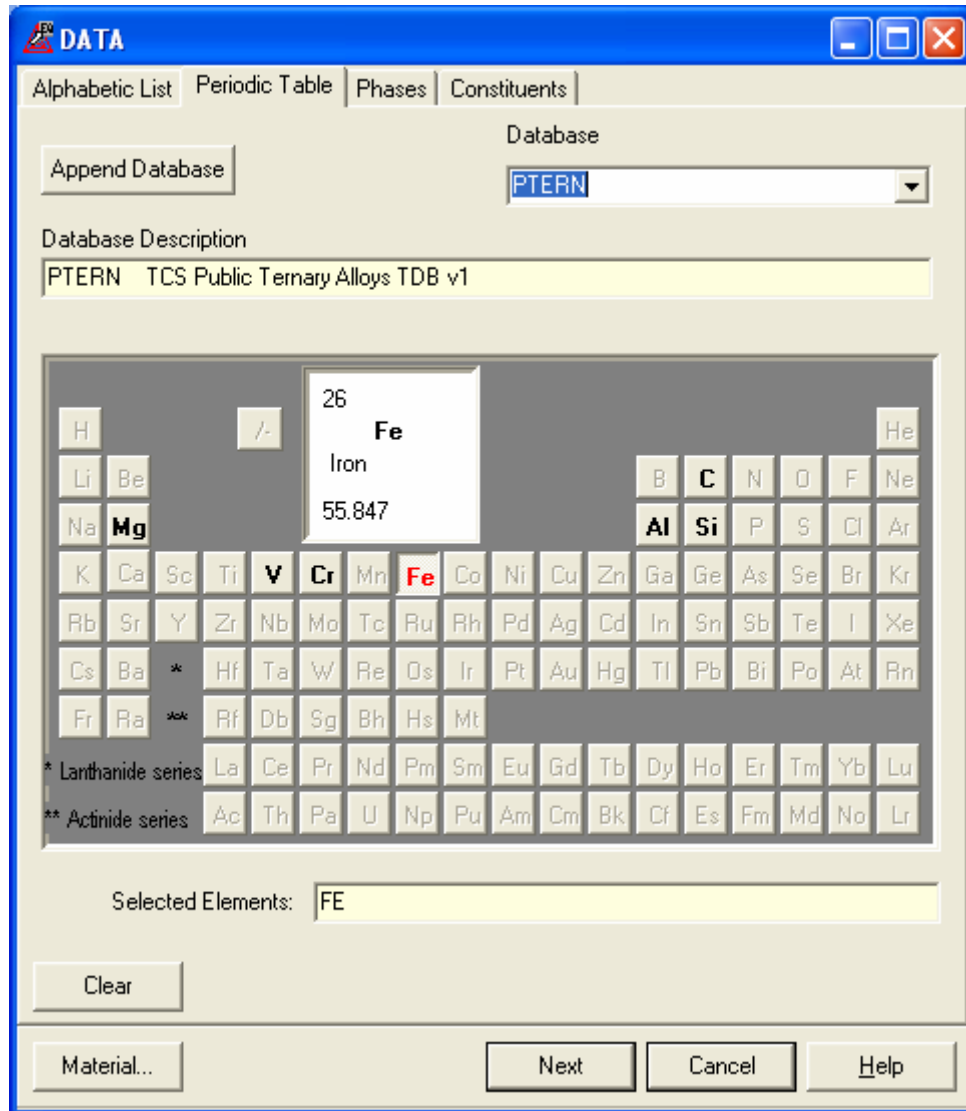


3. Select the elements *Fe* and *Cr* from the periodic table.
4. Click the *Phase Diagram* button.
5. The Fe-Cr binary phase diagram will be calculated and plotted automatically.



2 Plotting Thermodynamic Functions

1. Choose the *Elements* button in the MAIN window. Select *Fe* from the *PTERN* database. Press *Next*.



2. For a unary system, all conditions are already predefined when the CONDITIONS window opens. Accept the present conditions and press *Next*.

CONDITIONS

Number of Missing Conditions: 0

Temperature: 1000 K

Pressure: 101325 Pa

System Size: Moles, 1 moles

All Defined Conditions in SI Units:

```
T=1000
P=1.01325E5
N=1
```

Fixed Phases:

Buttons: Back..., Script Management..., Show Value..., Compute, Next, Cancel, Help

- Define axis 1 as T and axis 2 as $NONE$. Enter min and max values as 27 resp. 1700 K.
(The default temperature unit can be changed in the *Options* menu in the MAIN window.)
Click *Next* to start the stepping.

MAP/STEP DEFINITION

Axis 1:

Variable: T

Min (K): 27, No of steps: 50, Max (K): 1700

Axis 2:

Variable: NONE

Min (K): , No of steps: , Max (K):

Overwrite Previous Calculation: ☒ Step Separate: ☐

Generate Automatic Start Points: ☒

Buttons: Back..., Script Management..., Next, Cancel, Help

4. In order to plot thermodynamic functions for the individual phases, select the *User Symbols* tab in the DIAGRAM window and type in following four functions and one table, using the *Type*, *Name* and *Expression* boxes. Click *Add Symbol* after each definition.

Function $GF=GM(FCC)$

$GB=GM(BCC)$

$GH=GM(HCP)$

$GL=GM(LIQUID)$

Table $G1=GF,GB,GH,GL$

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | Advanced Diagram Axes

All Defined Symbols

```
GF=GM(FCC_A1)
GB=GM(BCC_A2)
GH=GM(HCP_A3)
GL=GM(LIQUID)
G1=GF,GB,GH,GL
```

Type: Table

Name:

Expression:

Add Symbol Delete Symbol Tabulate

X-Axis Text: ☒ Automatic
TEMPERATURE_KELVIN

Y-Axis Text: ☒ Automatic
NPM(*)

Back... ☐ New Graph Window Next Cancel Help

5. Open the *Advanced Diagram Axis* tab and choose the table G1 for the Y-axis. The X-axis needn't be changed. Click *Next* to plot.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | Advanced Diagram Axes

Diagram Title:

X-Axis

Temperature and Pressure: Temperature Kelvin

Potential and Activity:

Compositional Variables:

Phase Variables:

Energy Variables:

Additional Quantities:

Partial Derivatives:

User Symbols:

Y-Axis

Temperature and Pressure:

Potential and Activity:

Compositional Variables:

Phase Variables:

Energy Variables:

Additional Quantities:

Partial Derivatives:

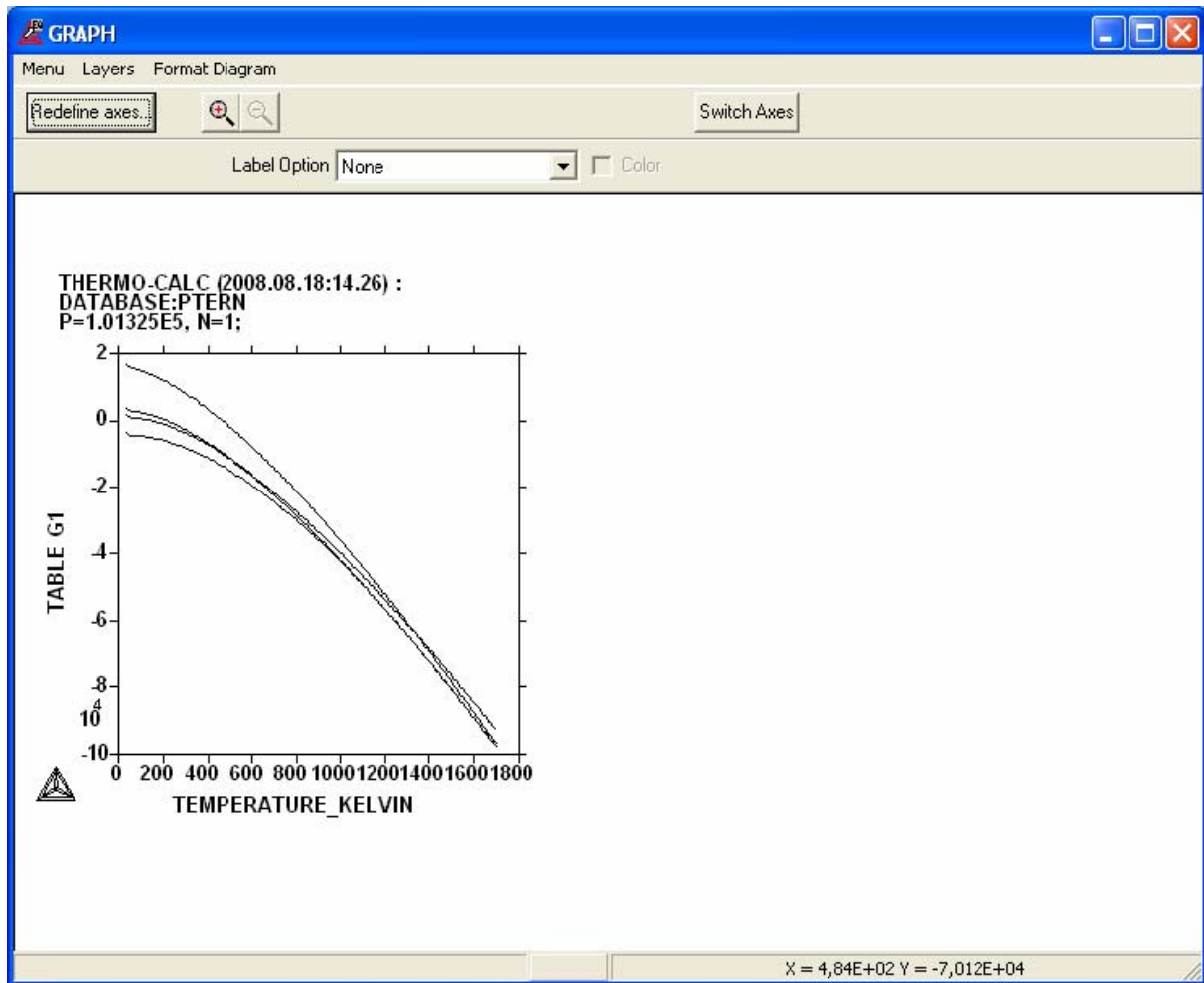
User Symbols: G1

X-Axis Text: ☒ Automatic
TEMPERATURE_KELVIN

Y-Axis Text: ☒ Automatic
TABLE G1

Back... ☐ New Graph Window Next Cancel Help

- Click *Redefine* to enter some other functions to make the small difference in Gibbs energy between the solution phases more visible.



- Type in new functions DGF , DGH , DGL which are the difference between the Gibbs energy for each phase compared with the Gibbs energy of the BCC phase. DGB will naturally be zero. Enter the functions in a table $G2$.

Function $DGF = GF - GB$
 $DGB = GB - GB$
 $DGH = GH - GB$
 $DGL = GL - GB$

Table $G2 = DGF, DGB, DGH, DGL$

Select *Advanced Diagram Axis* and change the Y-axis variable to $G2$ and click next to plot.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | Advanced Diagram Axes

All Defined Symbols

```
GF=GM(FCC_A1)
GB=GM(BCC_A2)
GH=GM(HCP_A3)
GL=GM(LIQUID)
DGF=GF-GB
DGB=GB-GB
DGH=GH-GB
DGL=GL-GB
G1=GF,GB,GH,GL
```

Type: Function Name: G2

Expression: DGF,DGB,DGH,DGL

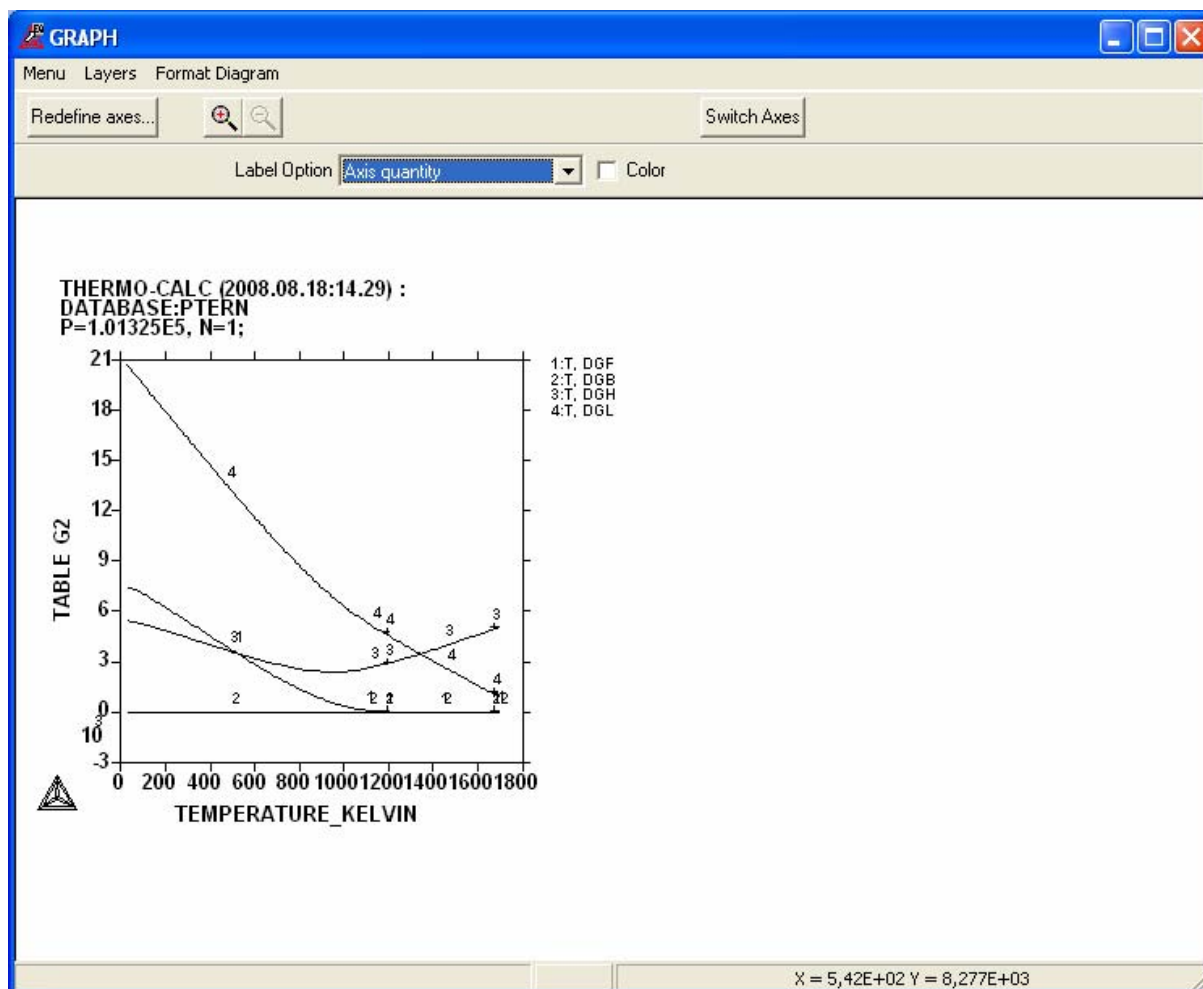
Add Symbol Delete Symbol Tabulate

X-Axis Text: ☒ Automatic Y-Axis Text: ☒ Automatic

TEMPERATURE_KELVIN NPM[°]

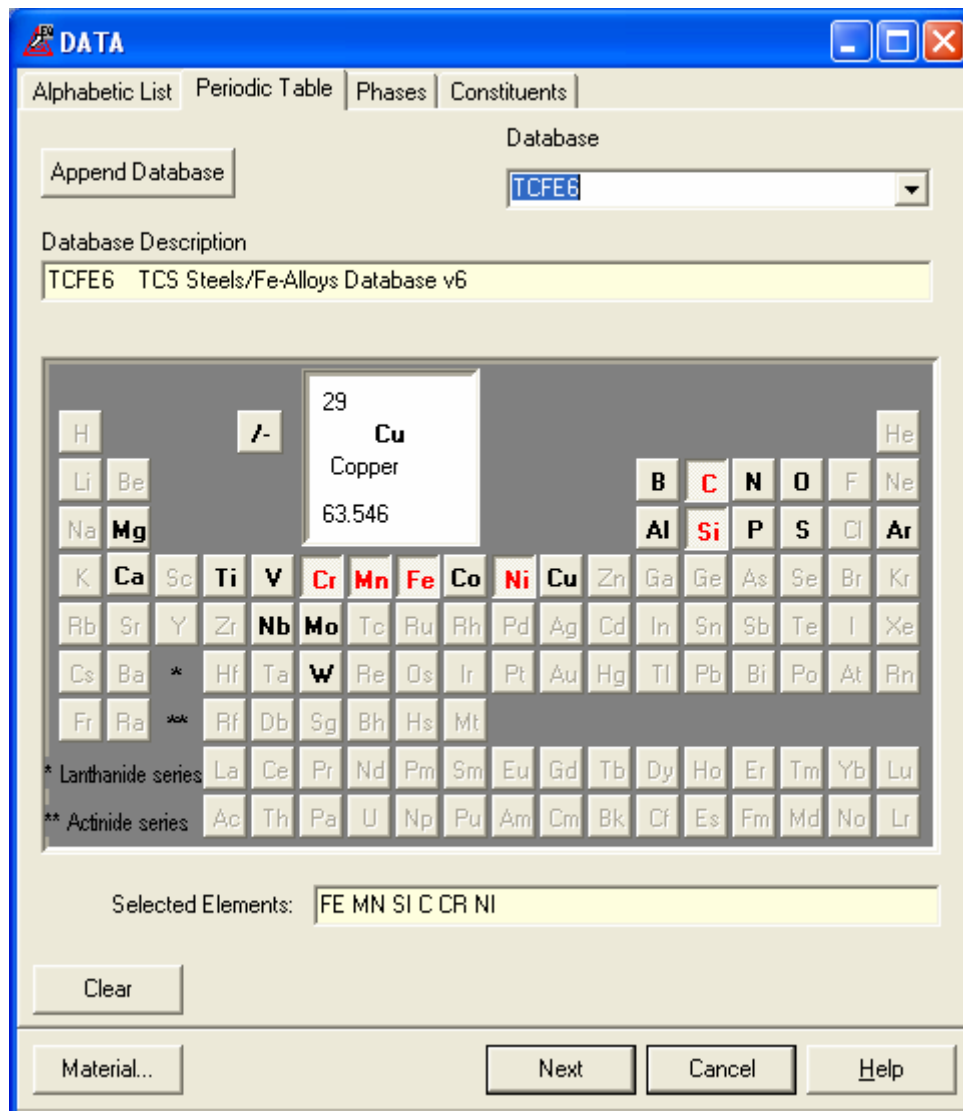
Back... ☐ New Graph Window Next Cancel Help

8. Select *Axis quantity* from the *Label Option* list.



3 Calculation of Single Equilibrium in Low Alloyed Fe-Mn-Si-Cr-Ni-C Steel

1. Start TCW and click *Elements* on the MAIN window.
2. In the DATA window, choose the *TCFE6* database and select the following six elements; Fe, Mn, Si, C, Cr, Ni. Finish by clicking *Next*.



3. To do an equilibrium calculation at 800 °C, enter this temperature in the *Temperature* box. (The default temperature unit can be changed in the *Options* menu in the MAIN window). Then enter the composition values in mass-percent for all the elements except the major Fe in the boxes on the right side of the CONDITIONS window: 0.4 Mn, 0.5 Si, 0.2 C, 1.5 Cr, and 3 Ni. Clicking *Next* will move you to the STEP/MAP DEFINITION window, choose instead *Compute* and look in the MAIN window.

CONDITIONS

Number of Missing Conditions: 0

Temperature: 800 C

Pressure: 101325 Pa

System Size: Moles 1 moles

All Defined Conditions in SI Units:

```
T=1073.15
P=1.01325E5
N=1
W(MN)=4E-3
W(SI)=5E-3
W(C)=2E-3
W(CR)=1.5E-2
W(NI)=3E-2
```

Fixed Phases:

Composition Unit: Mass-percent

Component	Value	Condition
FE		Composition
MN	0.4	Composition
SI	0.5	Composition
C	0.2	Composition
CR	1.5	Composition
NI	3	Composition

Buttons: Back... Script Management... Show Value... Compute Next Cancel Help

4. The result of this calculation is now shown in the MAIN window. The listing is equivalent to the output from the LIST-EQUILIBRIUM command in Thermo-Calc Classic. Under the present conditions, only fcc phase (austenite) is present as a stable phase. Note that the CONDITIONS window is still open for further calculations.

MAIN

File Edit Applications Script Options Window Help

Elements... Material...

Eq 1

Database: TCFE6

Conditions:
T=1073.15, P=1.01325E5, N=1, W(MN)=4E-3, W(SI)=5E-3, W(C)=2E-3, W(CR)=1.5E-2, W(NI)=3E-2
DEGREES OF FREEDOM 0

Temperature 1073K (800C, 1472F), Pressure 1,013250E+05
Number of moles of components 1,00000E+00, Mass 5,51867E+01
Total Gibbs energy -5,05909E+04, Enthalpy 2,94993E+04, Volume 7,17086E-06

Component	Moles	Mass-Fraction	Activity	Potential	Ref.State
C	9,1894E-03	2,0000E-03	3,5852E-02	-2,9698E+04	SER
CR	1,5920E-02	1,5000E-02	3,6447E-04	-7,0642E+04	SER
FE	9,3284E-01	9,4400E-01	4,7357E-03	-4,7760E+04	SER
MN	4,0181E-03	4,0000E-03	5,3430E-06	-1,0832E+05	SER
NI	2,8209E-02	3,0000E-02	6,9330E-05	-8,5450E+04	SER
SI	9,8246E-03	5,0000E-03	1,2756E-09	-1,8274E+05	SER

FCC_A1#1 STATUS ENTERED Driving force 0,0000E+00
Number of moles 1,0000E+00, Mass 5,5187E+01
Mass fractions:
FE 9,44000E-01 CR 1,50000E-02 MN 4,00000E-03
NI 3,00000E-02 SI 5,00000E-03 C 2,00000E-03

5. A more interesting calculation is to find out at what temperature bcc (ferrite) becomes stable for this steel (the A3 line). Go back to the CONDITIONS window and take away the condition on temperature (mark $T=800$ in the list and click *Delete*, or clear the *Temperature* box). The degrees of freedom will change from zero to one.

CONDITIONS

Number of Missing Conditions: 1

Temperature: C

Pressure: 101325 Pa

System Size: Moles 1 moles

All Defined Conditions in SI Units

```
P=1.01325E5
N=1
W(MN)=4E-3
W(SI)=5E-3
W(C)=2E-3
W(CR)=1.5E-2
W(NI)=3E-2
```

Delete

Fixed Phases

Set Reference State | User Symbols | Start Values

Components | Advanced Conditions | Phases

Composition Unit: Mass-percent

Component	Value	Condition
FE	<input type="text"/>	Composition
MN	0.4	Composition
SI	0.5	Composition
C	0.2	Composition
CR	1.5	Composition
NI	3	Composition

Redefine...

Back... Script Management... Show Value... Compute Next Cancel Help

6. Now select the *Phases* tab on the right hand side of the window. Click the *BCC_A2* phase and select the status *FIXED* in the *Phase Status* box. Type the value 0 (zero) in the box right next to it. This will specify that the bcc phase must take part in the equilibrium, which changes the degrees of freedom back to zero again. Zero amount of the bcc phase will find the bcc/bcc+fcc phase diagram line, which is where bcc start to form. Press *Compute*.

CONDITIONS

Number of Missing Conditions: 0

Temperature: C

Pressure: 101325 Pa

System Size: Moles 1 moles

All Defined Conditions in SI Units:

```
P=1.01325E5
N=1
W(MN)=4E-3
W(SI)=5E-3
W(C)=2E-3
W(CR)=1.5E-2
W(NI)=3E-2
```

Delete

Fixed Phases:

```
BCC_A2 = 0.00
```

Set Reference State | User Symbols | Start Values

Components | Advanced Conditions | Phases

Phases	Status	Moles
LIQUID	ENTERED	0.00
AL4C3	ENTERED	0.00
BCC_A2	FIXED	0.00
CEMENTITE	ENTERED	0.00
CHI_A12	ENTERED	0.00
CR3SI	ENTERED	0.00
DIAMOND_FCC_A4	ENTERED	0.00
FCC_A1	ENTERED	1.00
FCC_A1#2	ENTERED	0.00
FE2SI	ENTERED	0.00
FE4N_LP1	ENTERED	0.00
FE8SI2C	ENTERED	0.00
FECN_CHI	ENTERED	0.00
GRAPHITE	ENTERED	0.00

Phase Status:

FIXED 0.00 moles

Phase Conditions...

Add Composition Set...

Back... Script Management... Show Value... Compute Next Cancel Help

7. The new equilibrium is shown in the MAIN window. Use the scrollbar to view the entire listing. The A3 temperature for this steel is 756 °C.

MAIN

File Edit Applications Script Options Window Help

Elements... Material...

Eq 2

Conditions:
P=1.01325E5, N=1, W(MN)=4E-3, W(SI)=5E-3, W(C)=2E-3, W(CR)=1.5E-2, W(NI)=3E-2
DEGREES OF FREEDOM 0


Temperature 1029K (756C, 1393F), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass 5.51867E+01
Total Gibbs energy -4.73427E+04, Enthalpy 2.80653E+04, Volume 7.15074E-06

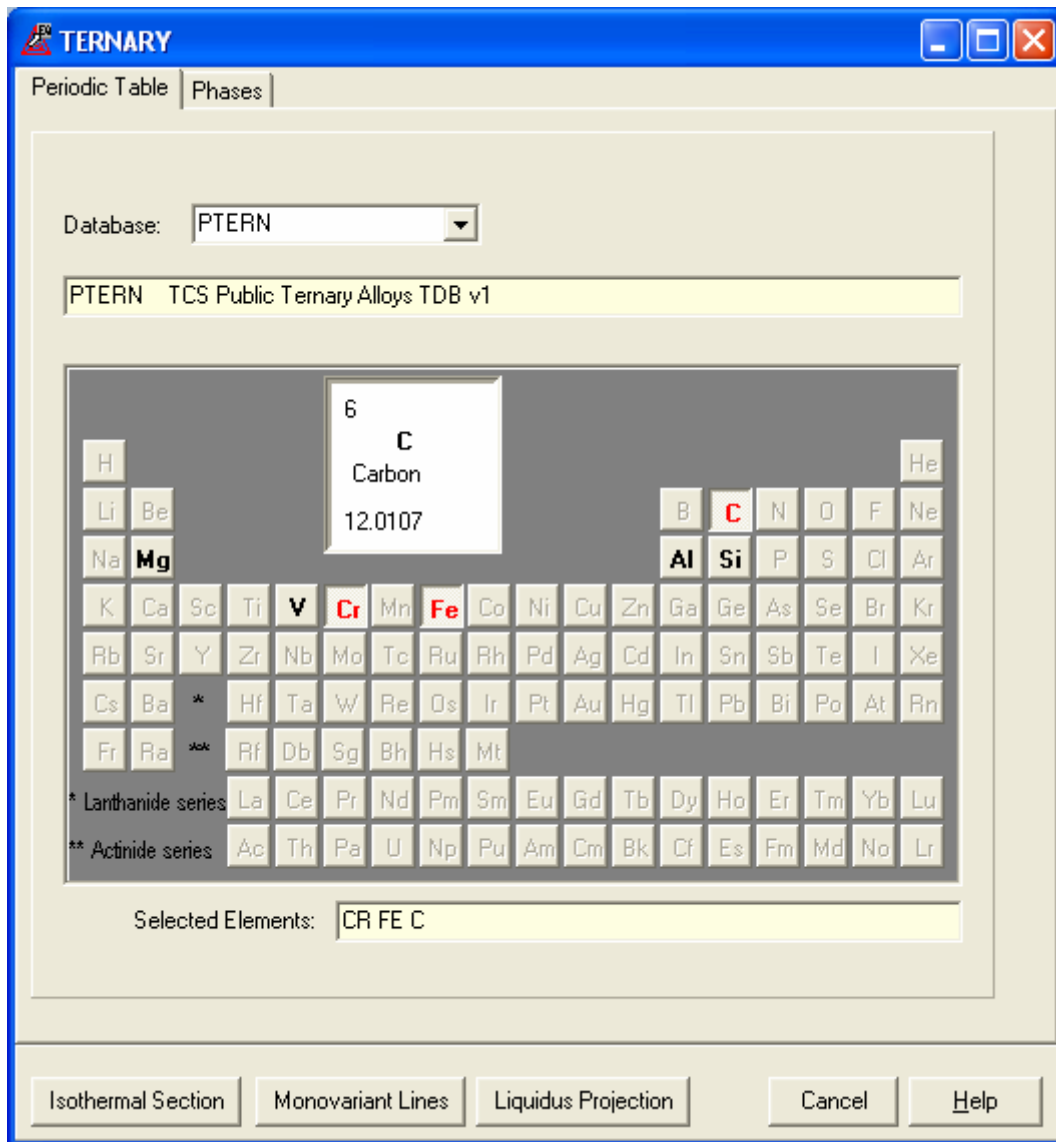
Component	Moles	Mass-Fraction	Activity	Potential	Ref.State
C	9.1894E-03	2.0000E-03	4.6760E-02	-2.6209E+04	SER
CR	1.5920E-02	1.5000E-02	4.3309E-04	-6.6274E+04	SER
FE	9.3284E-01	9.4400E-01	5.4708E-03	-4.4570E+04	SER
MN	4.0181E-03	4.0000E-03	5.8404E-06	-1.0312E+05	SER
NI	2.8209E-02	3.0000E-02	7.6121E-05	-8.1153E+04	SER
SI	9.8246E-03	5.0000E-03	7.5297E-10	-1.7977E+05	SER

BCC_A2#1 STATUS FIXED Driving force 0.0000E+00
Number of moles 0.0000E+00, Mass 0.0000E+00
Mass fractions:
FE 9.67624E-01 CR 1.10444E-02 MN 1.36701E-03
NI 1.39622E-02 SI 5.94913E-03 C 5.35070E-05

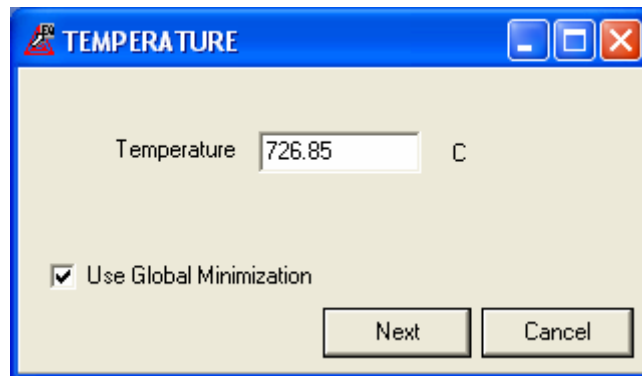
FCC_A1#1 STATUS ENTERED Driving force 0.0000E+00
Number of moles 1.0000E+00, Mass 5.5187E+01
Mass fractions:
FE 9.44000E-01 CR 1.50000E-02 MN 4.00000E-03
NI 3.00000E-02 SI 5.00000E-03 C 2.00000E-03

4 Isothermal Section of the Fe-Cr-C System at 1000 K

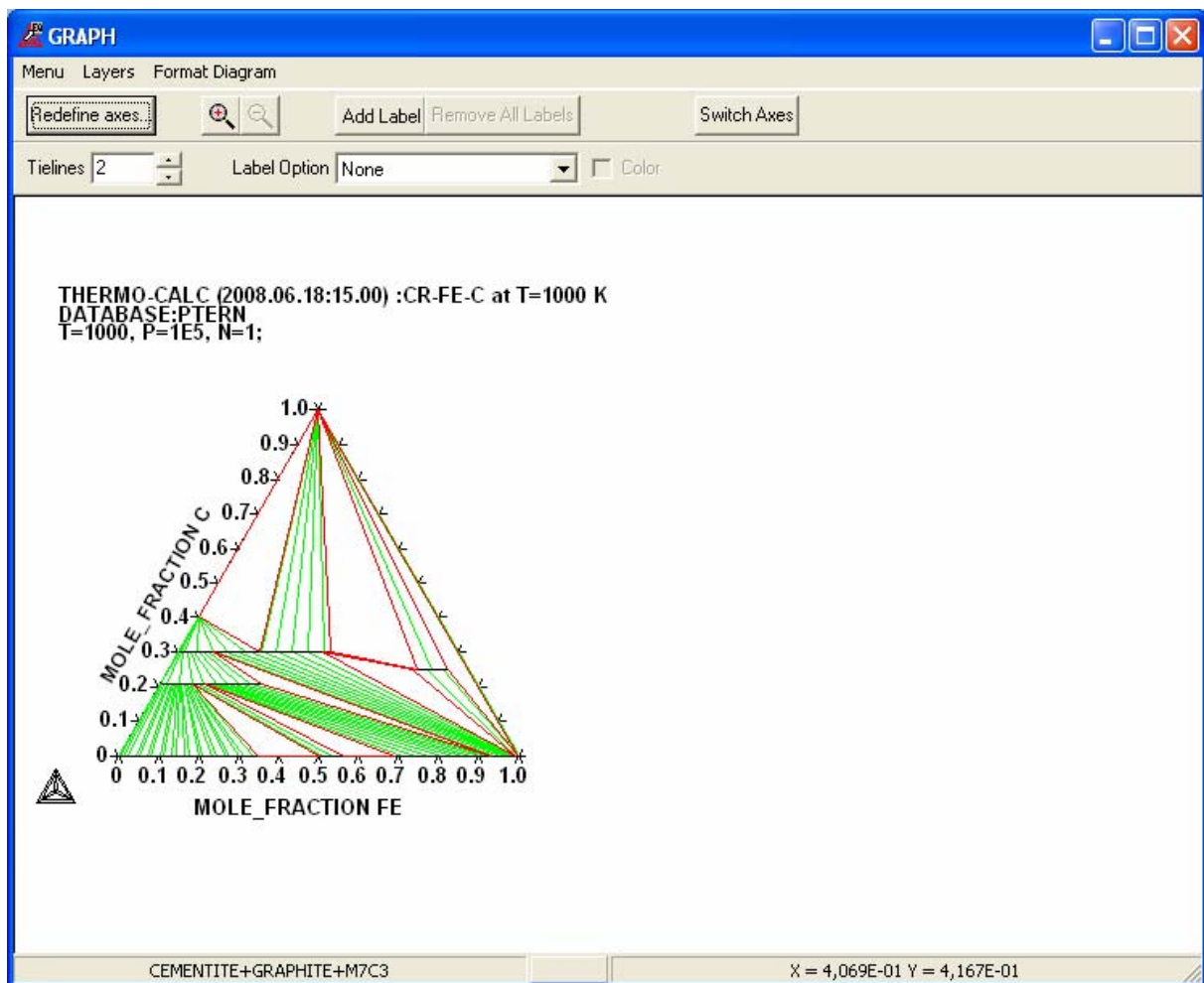
1. Here we use the ternary module in TCW, which is opened by clicking 
2. Select the *PTERN* database in the *Database* box and click the three elements in the periodic table; Cr, Fe, and C.
3. Click *Isothermal Section* to continue.



4. When the temperature box appears the temperature is set to 726.85 °C (1000 K). The default unit may be changed to K in the *Options/Units* menu in the MAIN window. Click *Next* to proceed.



5. To plot the isothermal section click *next*. By placing the mouse cursor at a certain region in the diagram the name of the phase(s) stable in that region is displayed in the lower left corner of the GRAPH window.



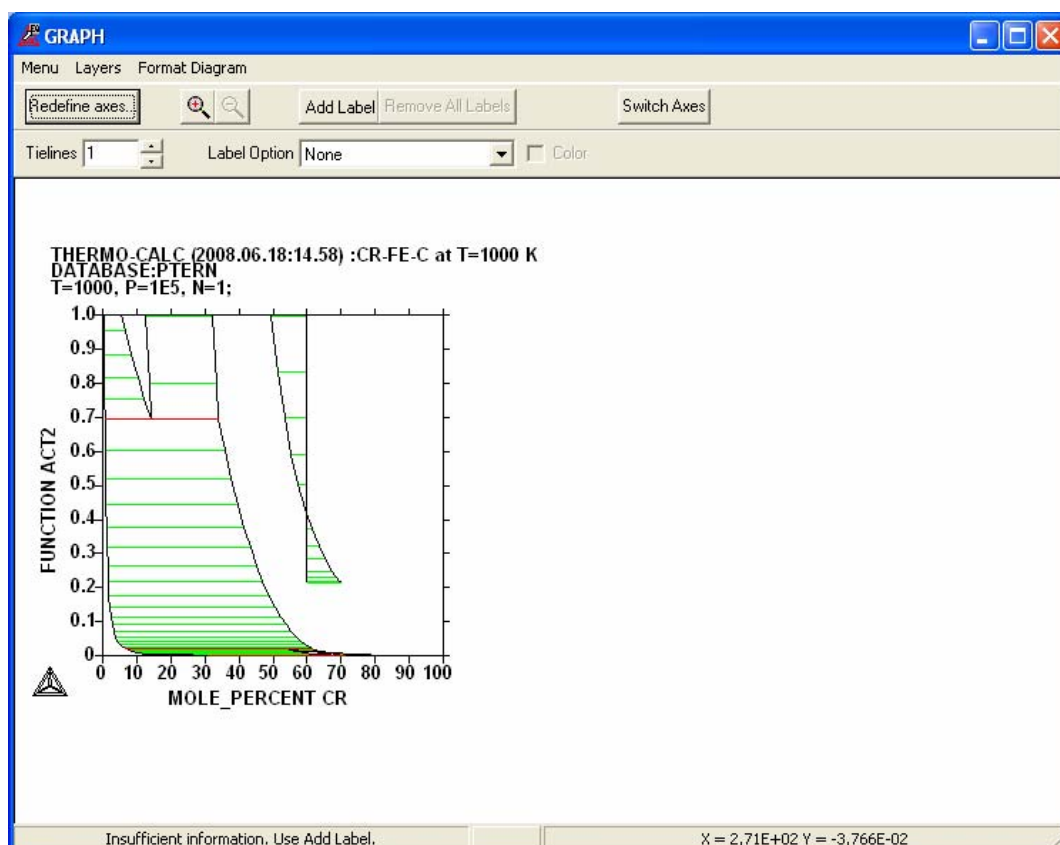
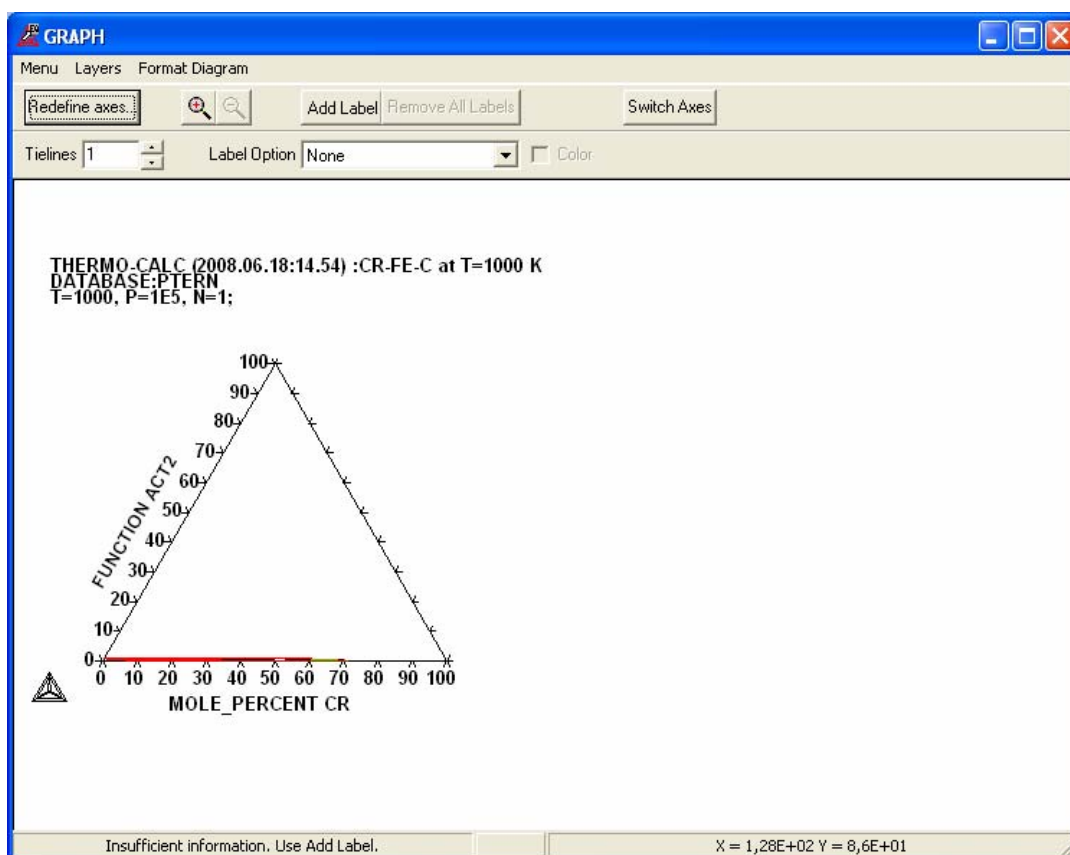
- Press *Redefine* to plot amount of Cr vs. activity of carbon instead. To get easily understandable activity values, open the User Symbols tab and enter a function for the activity of carbon referred to the current temperature: $ACT2=ACR(C,GRAPHITE)$.

The 'DIAGRAM DEFINITION' dialog box is shown with the 'User Symbols' tab selected. The 'All Defined Symbols' list contains the function $ACT2=ACR(C,GRAPHITE)$. Below this, the 'Type' is set to 'Function' and the 'Name' field is empty. The 'Expression' field is also empty. At the bottom, the 'X-Axis Text' is 'MOLE_FRACTION FE' and the 'Y-Axis Text' is 'MOLE_FRACTION C', both with the 'Automatic' checkbox checked. The 'Back...', 'Next', 'Cancel', and 'Help' buttons are visible at the bottom.

- Next select *Advanced Diagram Axis* and set the X-Axis variable to Mass Percent Cr and the Y-Axis variable to the function ACT2. Click next to plot.

The 'DIAGRAM DEFINITION' dialog box is shown with the 'Advanced Diagram Axes' tab selected. The 'Diagram Title' is 'CR-FE-C at T=1000 K'. The 'X-Axis' section has 'Compositional Variables' set to 'Mole-percent' and 'For Component' set to 'CR'. The 'Y-Axis' section has 'User Symbols' set to 'ACT2'. At the bottom, the 'X-Axis Text' is 'MOLE_PERCENT CR' and the 'Y-Axis Text' is 'FUNCTION ACT2', both with the 'Automatic' checkbox checked. The 'Back...', 'Next', 'Cancel', and 'Help' buttons are visible at the bottom.

8. Change the type of diagram from triangular to normal using the *Format Diagram* menu.



5 Calculation of Isopleth in Fe-8Cr-1C System

1. Open the TCW program.
2. Click *Elements*.
3. Select *PTERN* from the *Database* list and then click alloy elements *C*, and *Cr*, and *Fe* in the periodic table. Click *Next*.
4. Specify the concentrations of C and Cr as *1* and *8 mass-percent*, respectively and accept the default temperature. Click *Next*.

CONDITIONS

Number of Missing Conditions: 0

Temperature: 1000 K

Pressure: 101325 Pa

System Size: Moles, 1 moles

All Defined Conditions in SI Units:

```
T=1000
P=1.01325E5
N=1
W(C)=1E-2
W(CR)=8E-2
```

Delete

Fixed Phases:

Set Reference State: Components

User Symbols: Advanced Conditions

Start Values: Phases

Composition Unit: Mass-percent

Component	Value	Condition
C	1	Composition
CR	8	Composition
FE		Composition

Back... Script Management... Show Value... Compute Next Cancel Help

5. The default mapping axis, $W(C)$ and T are just what we are interested in and the minimum and maximum values for them are OK. Click *Next*.

MAP/STEP DEFINITION

Axis 1

Variable:

Min (%): No of steps: Max (%):

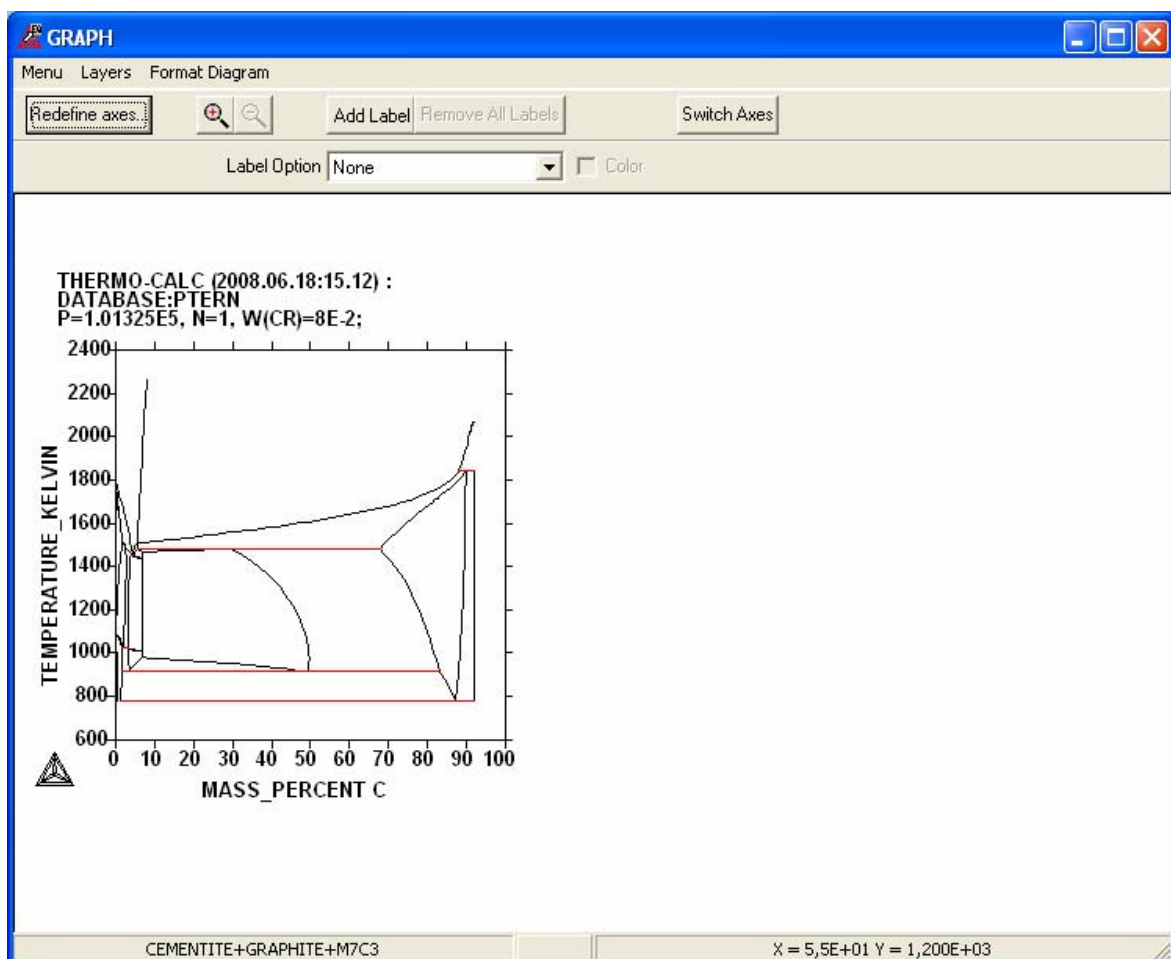
Axis 2

Variable:

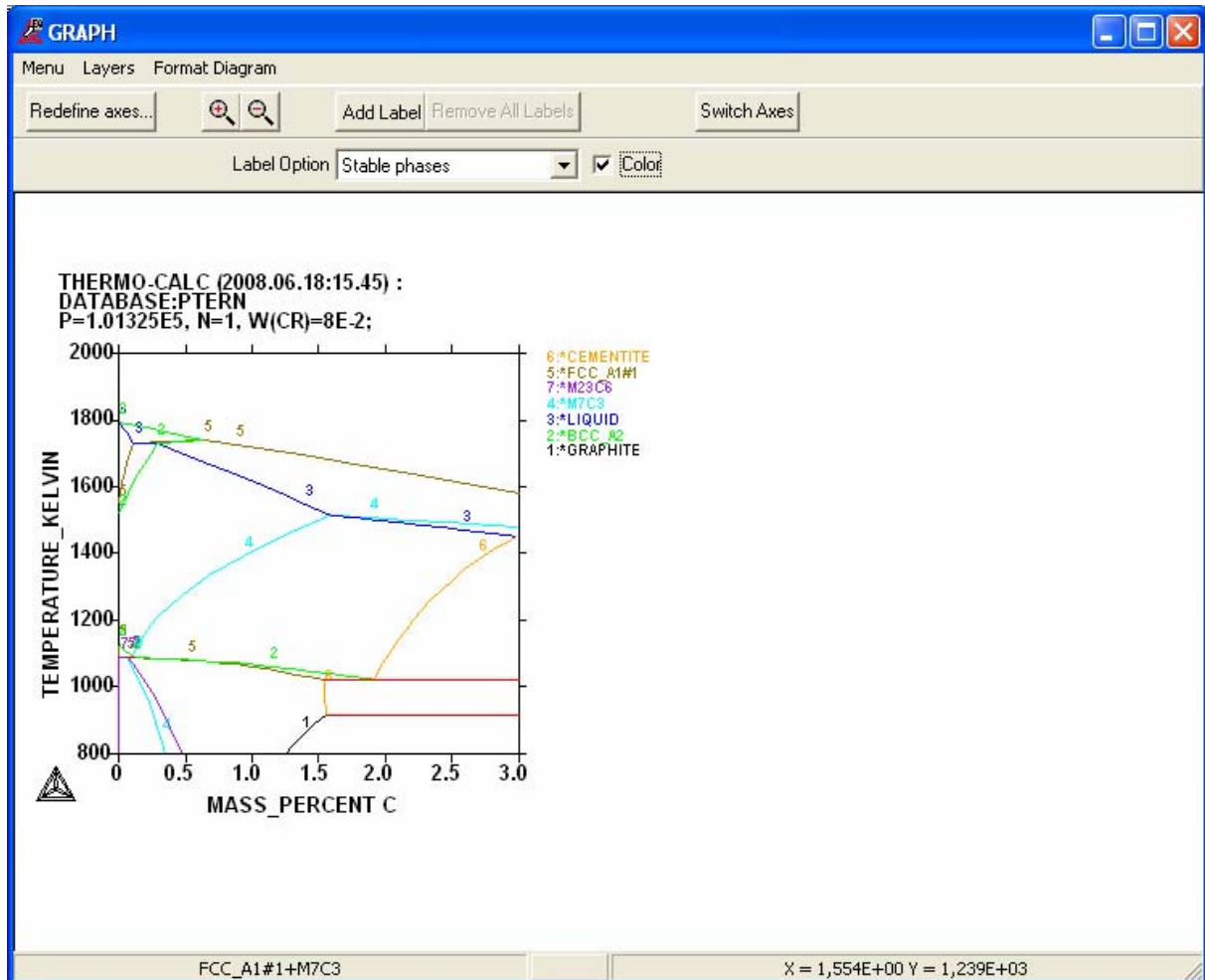
Min (K): No of steps: Max (K):

☒ Overwrite Previous Calculation ☐ Step Separate
☒ Generate Automatic Start Points

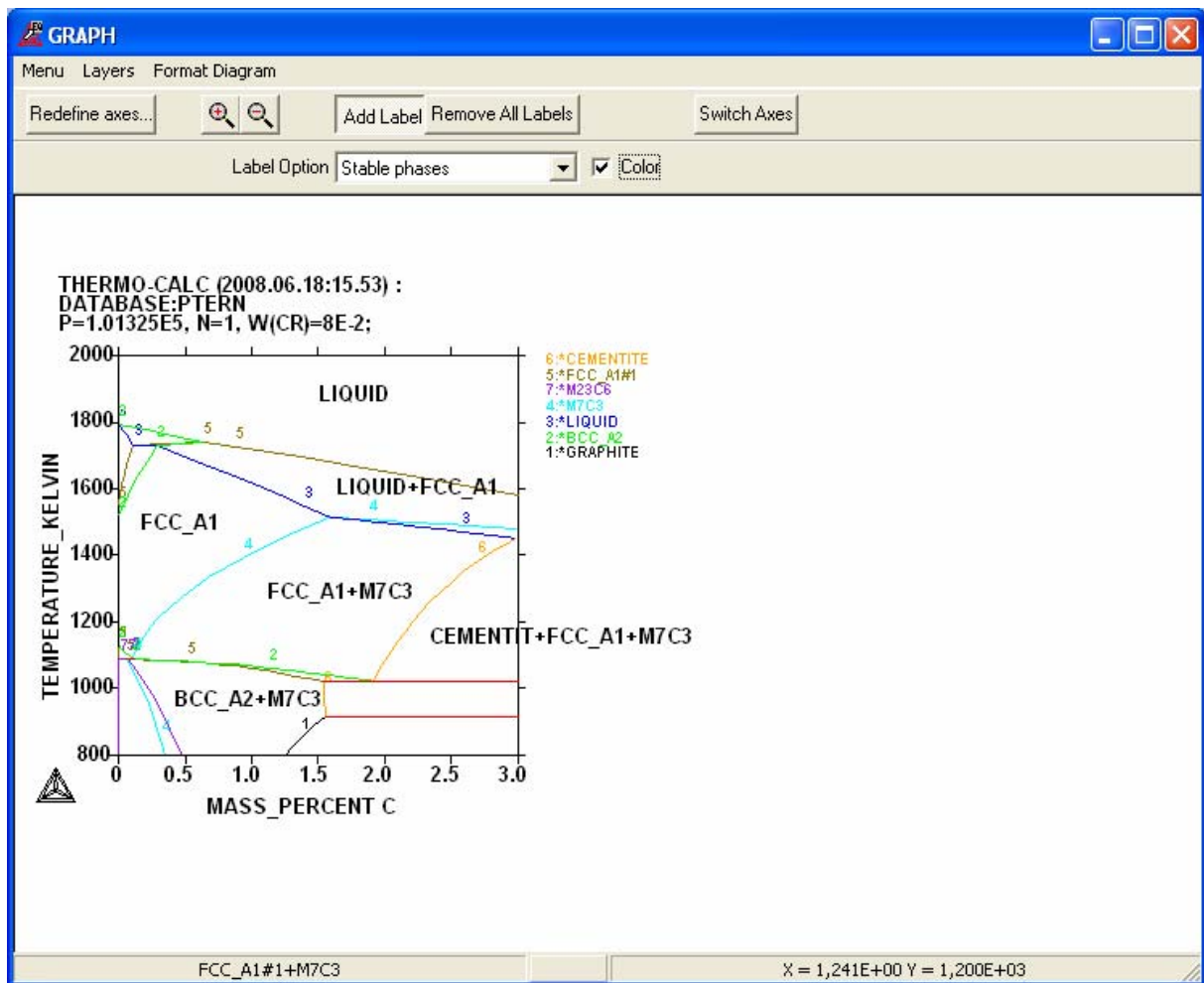
6. After the calculation is finished, the DIAGRAM DEFINITION window pops up. The mapping axes are shown as the default plotting X-axis and Y-axis now. Click *Next*. The following diagram is plotted.



7. Choose *Scaling* from the *Format Diagram* menu to open the Scaling tab on the DIAGRAM DEFINITION window. Specify the min value for X-axis as 0 and max as 3, and for Y-axis as 800 and 2000. Click *Next*.
8. Select *Stable phases* in the *Label Option* menu and check the color box.



9. The phase regions can also be labeled by first clicking *Add Label* and then clicking in the phase fields you want to label. In the following diagram, the *Liquid*, *Fcc_A1*, *Liquid+Fcc_A1*, *Fcc_A1+M7C3*, *Cementite+Fcc_A1+M7C3*, *Bcc_A2+M7C3* phase regions have been labeled.



6 Calculation of a Vertical Section for Mixing of Fe-1Cr-0.1C and Fe-20Cr-2C Alloys

1. Open the TCW program.
2. Click *Elements*.
3. Select *PTERN* from the *Database* list and then click alloy elements *Fe*, *C*, and *Cr* in the periodic table. Click *Next*.
4. A vertical section across the Fe-1Cr-0.1C and Fe-20Cr-2C alloys can be mapped by varying either Cr or C content and temperature and keeping the constraint condition between W(CR) and W(C): $W(\text{CR})/W(\text{C}) = (20-1)/(2-0.1) = 19/1.9 = 10$, i.e. $W(\text{CR}) - 10W(\text{C}) = 0$. Supposing we are varying Cr content, first set an arbitrary concentration of Cr between these two alloys, say 15, then click the *Advanced Conditions* tab, enter the equation $W(\text{CR}) - 10W(\text{C}) = 0$ in the *User Defined Conditions* box. Click *Next*.

CONDITIONS

Number of Missing Conditions: 1

Temperature: 1000 K

Pressure: 101325 Pa

System Size: Moles, 1 moles

All Defined Conditions in SI Units:

```
T=1000
P=1.01325E5
N=1
W(CR)=0.15
```

Delete

Fixed Phases:

Set Reference State: Components

User Symbols: Advanced Conditions

Start Values: Phases

Composition Unit: Mass-percent

Component	Value	Condition
FE		Composition
C		Composition
CR	15	Composition

Redefine...

Back... Script Management... Show Value... Compute Next Cancel Help

CONDITIONS

Number of Missing Conditions: 1

Temperature: 1000 K

Pressure: 101325 Pa

System Size: Moles, 1 moles

All Defined Conditions in SI Units:

```
T=1000
P=1.01325E5
N=1
W(CR)=0.15
```

Fixed Phases:

User Defined Conditions:

$$W(CR) - 10W(C) = 0$$

Normalization:

Property	Unit
Gibbs Energy	J/mol
Helmholtz Energy	J/mol
Enthalpy	J/mol
Entropy	J/mol/K
Volume	m ³ /mol

Buttons: Back..., Script Management..., Show Value..., Compute, Next, Cancel, Help

- Define the mapping ranges: from 0 to 20%Cr and 600 to 1900 K. Click *Next*.

MAP/STEP DEFINITION

Axis 1:

Variable: W(CR)

Min (%): 0, No of steps: 50, Max (%): 20

Axis 2:

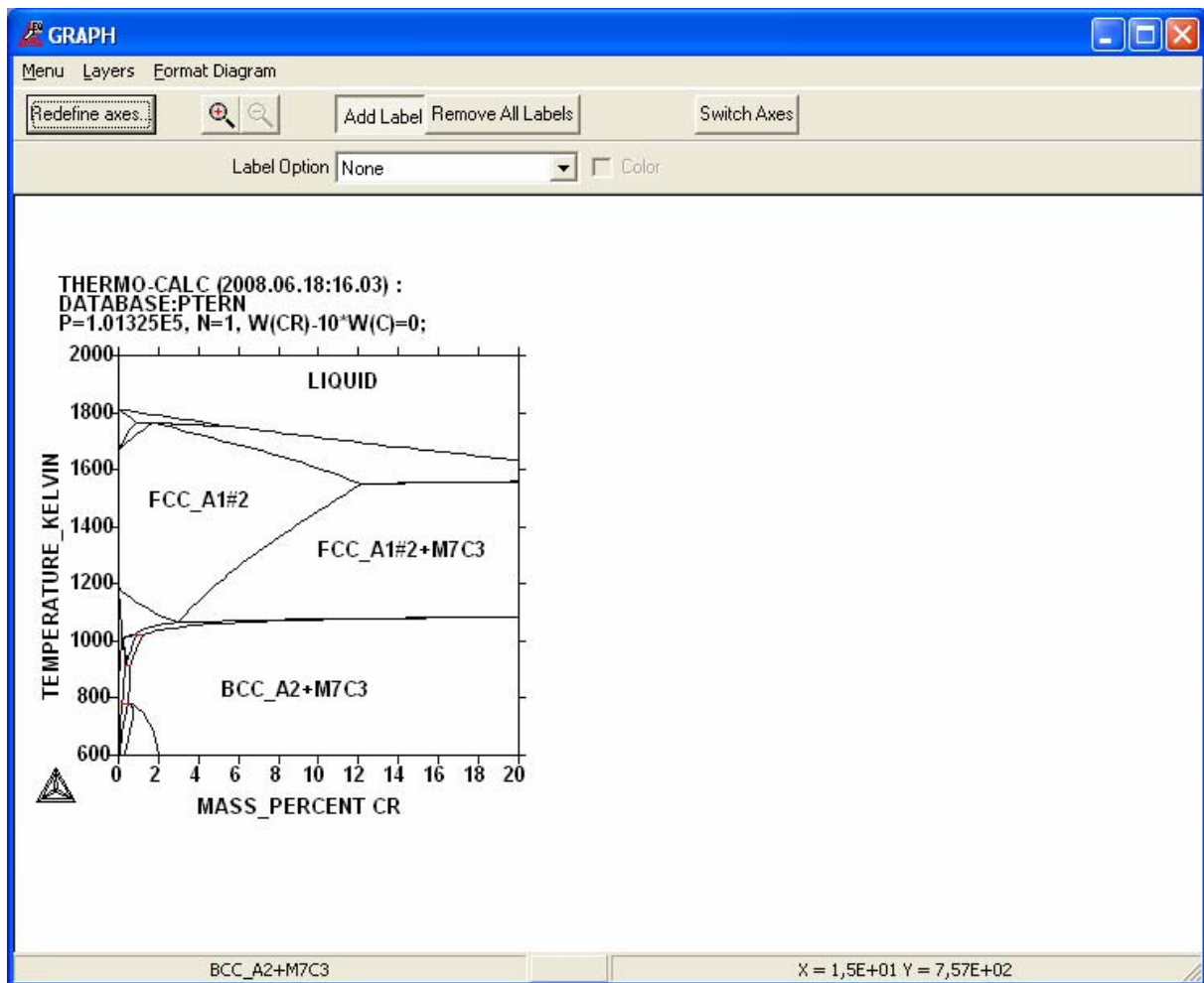
Variable: T

Min (K): 600, No of steps: 50, Max (K): 1900

☒ Overwrite Previous Calculation
 ☐ Step Separate
 ☒ Generate Automatic Start Points

Buttons: Back..., Script Management..., Next, Cancel, Help

- Click *Next* and the vertical section is plotted. One can label phase regions by first clicking *Add Label* and clicking in the phase regions one wants to label. The following is a labeled diagram.



7. Of course, one can now also plot C wt.% vs T. Click *Redefine* to change the X-Axis.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | Advanced Diagram Axes

Temperature Unit

☐ Celsius

☒ Kelvin

☐ Fahrenheit

Composition Unit

☐ Moles

☒ Percent

☒ Mass

Diagram Title

X-Axis

Variable

Composition

For Component

C

For Phase

SYSTEM

Y-Axis

Variable

Temperature

For Component

NONE

For Phase

SYSTEM

X-Axis Text

☒ Automatic

MASS_PERCENT C

Y-Axis Text

☒ Automatic

TEMPERATURE_KELVIN

Back...

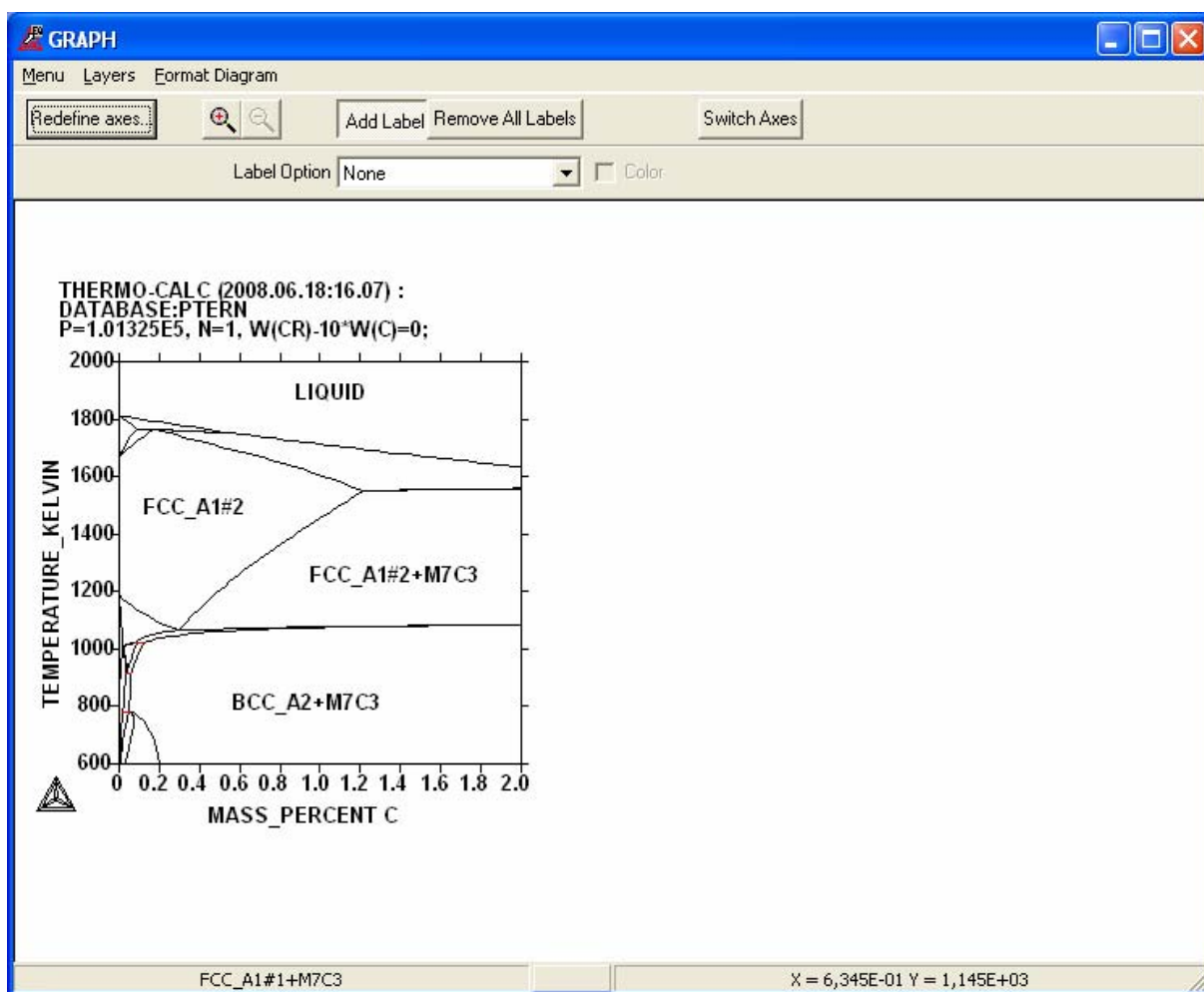
☐ New Graph Window

Next

Cancel

Help

8. Click *Next* and the vertical section is plotted. The following is a labeled diagram.



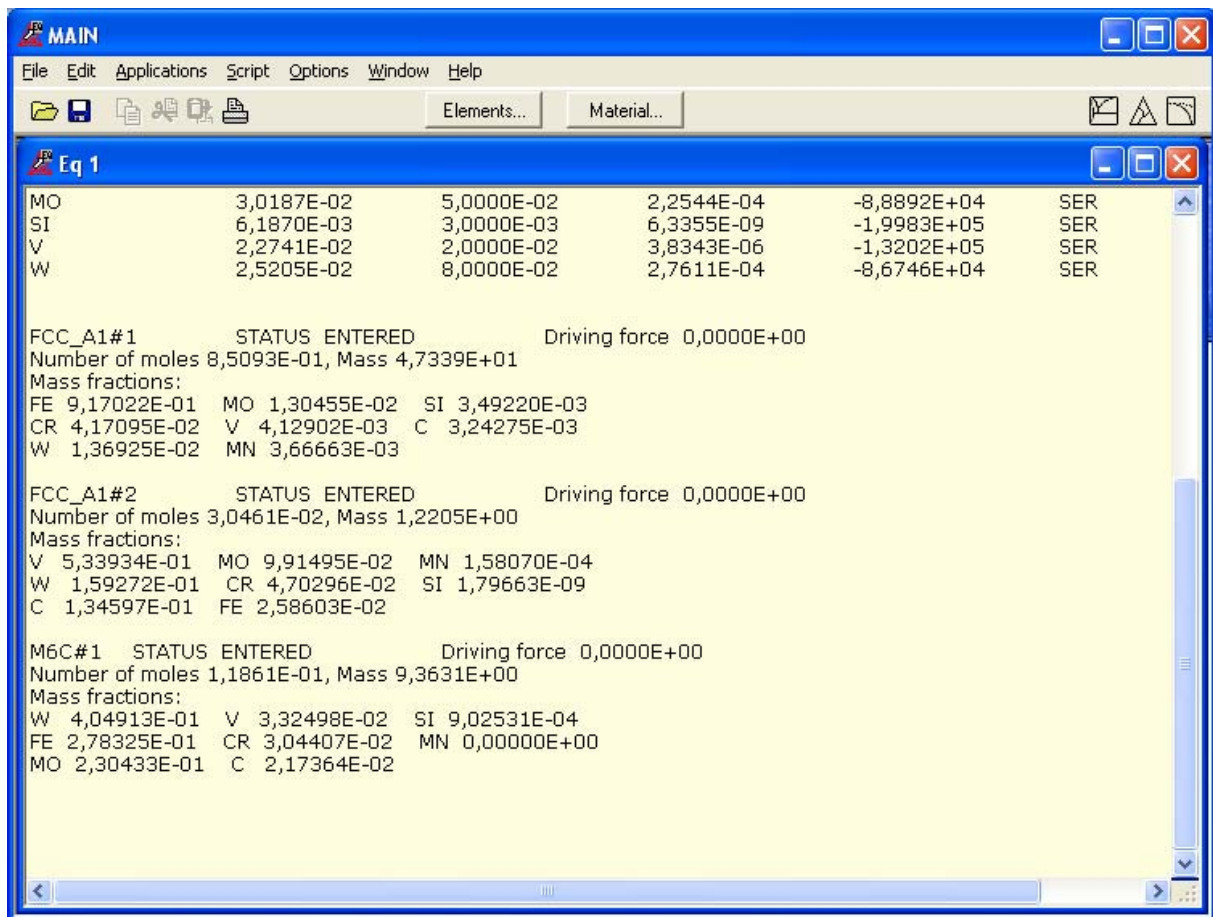
7 Calculation of Property Diagram of a High Speed Steel

1. Click the *Elements* button in the MAIN window, and select *TCFE6* in the *Database* box in the DATA window. Select the eight elements Fe, C, Cr, Si, Mn, W, Mo and V. Then click *Next*.
2. Define a single equilibrium in the CONDITIONS window. Put the temperature to *1000 °C* (the default settings for the temperature unit can be changed under the *Options* menu in the MAIN window), and the compositions to *0.9 % C*, *4 % Cr*, *0.3 % Mn*, *5 % Mo*, *0.3 % Si*, *2 % V* and *8 % W* (mass %). Fe is the balance, leave the box empty. Now click *Next*.

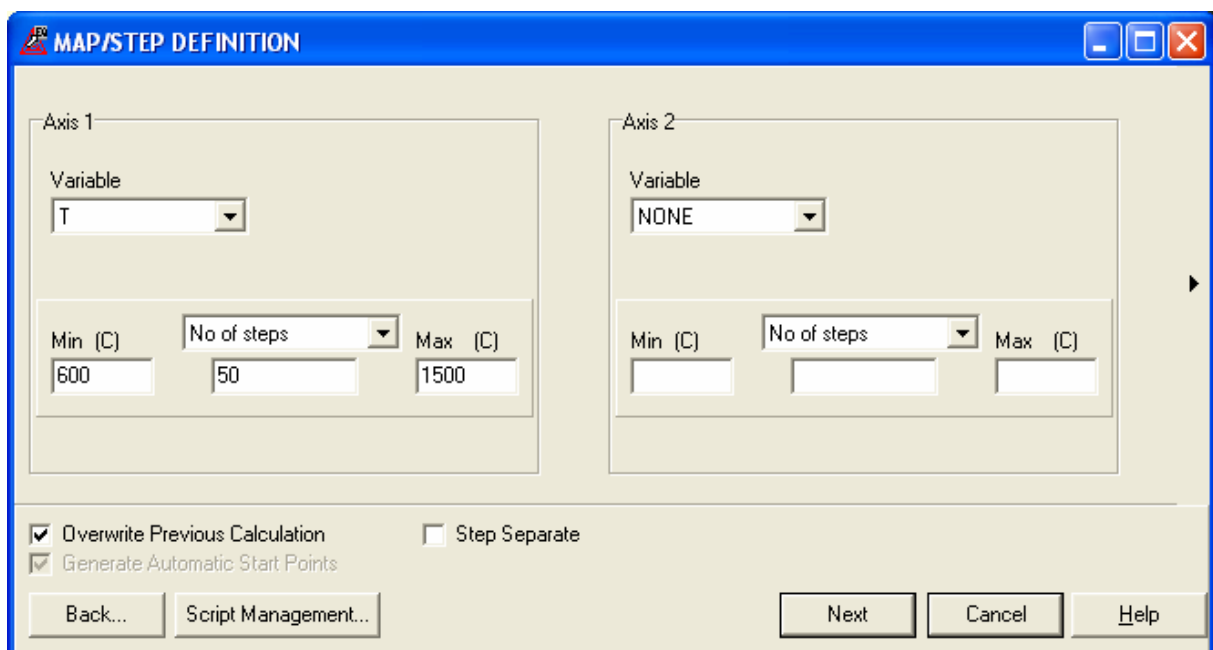
The screenshot shows the 'CONDITIONS' window in THERM-CALC. The 'Set Reference State' tab is active. The 'Components' section lists the elements: FE, C, CR, SI, MN, W, MO, and V. The 'Value' column shows the mass percentages: 0.9, 4, 0.3, 0.3, 8, 5, and 2 respectively. The 'Condition' column for all elements is set to 'Composition'. The 'Composition Unit' is set to 'Mass-percent'. The 'Temperature' is set to 1000 °C and 'Pressure' is 101325 Pa. The 'System Size' is set to 'Moles' with a value of 1. The 'All Defined Conditions in SI Units' list shows the calculated equilibrium conditions: T=1273.15, P=1.01325E5, N=1, and various weight fractions (W) for each element. The 'Fixed Phases' section is empty. The bottom buttons include 'Back...', 'Script Management...', 'Show Value...', 'Compute', 'Next', 'Cancel', and 'Help'.

Component	Value	Condition
FE		Composition
C	0.9	Composition
CR	4	Composition
SI	0.3	Composition
MN	0.3	Composition
W	8	Composition
MO	5	Composition
V	2	Composition

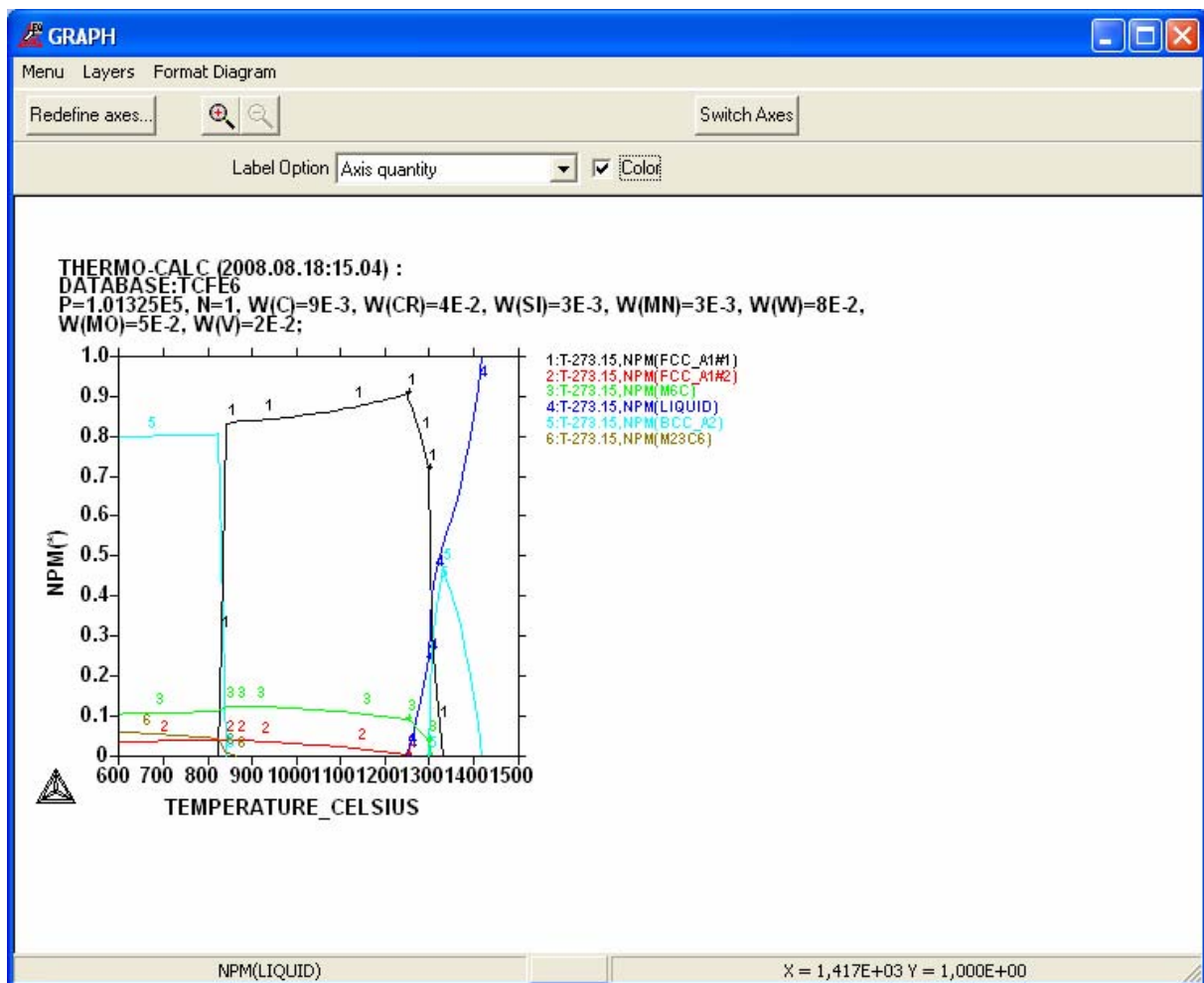
3. Before the axes are defined in the MAP/STEP window, it is useful to take a look at the calculated equilibrium in the MAIN window to see that it is reasonable. In this case we have a metallic fcc phase (85 mole percent) and two carbides: FCC_A1#2 and M6C. The second fcc phase is a MC carbide with mostly vanadium on the metal sublattice. Tungsten is the majority element in the M6C phase.



- The most common property diagram calculation is obtained by stepping in temperature for a given composition. Various temperature dependent quantities can then be used on the Y-axis in the DIAGRAM DEFINITION window. Change axis 1 to *T* and axis 2 to *NONE*. The limits for the temperature axis can be 600 – 1500 °C. Click *Next*.



- When the step calculation is finished, the DIAGRAM DEFINITION window appears with two axes already defined, let's use these. Press *Next*.
- Select *Axis quantity* in the *Label Option* menu and check the color box. The y-axis quantity means the fraction of each phase expressed in moles. We can see that in addition to the phases stable at $T=1000\text{ }^{\circ}\text{C}$, also bcc and M23C6 are stable at low temperature and liquid at high T. The cursor can be used to get an estimate of the values in the diagram. In the plot window below the cursor is placed on the liquidus temperature, $1417\text{ }^{\circ}\text{C}$.



- Another example of a property diagram is the activity of carbon vs. temperature. Click *Redefine* and open the *Advanced Diagram Axis* tab. Change the Y-axis variable to *Activity* for component C. Click *Next* to plot.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | Advanced Diagram Axes

Diagram Title

X-Axis

Temperature and Pressure: **Temperature Celsius**

Potential and Activity: **Activity**

Compositional Variables: **Activity**

Phase Variables: **Activity**

Energy Variables: **Activity**

Additional Quantities: **Activity**

Partial Derivatives: **Activity**

User Symbols: **Activity**

Y-Axis

Temperature and Pressure: **Activity**

Potential and Activity: **Activity**

Compositional Variables: **Activity**

Phase Variables: **Activity**

Energy Variables: **Activity**

Additional Quantities: **Activity**

Partial Derivatives: **Activity**

User Symbols: **Activity**

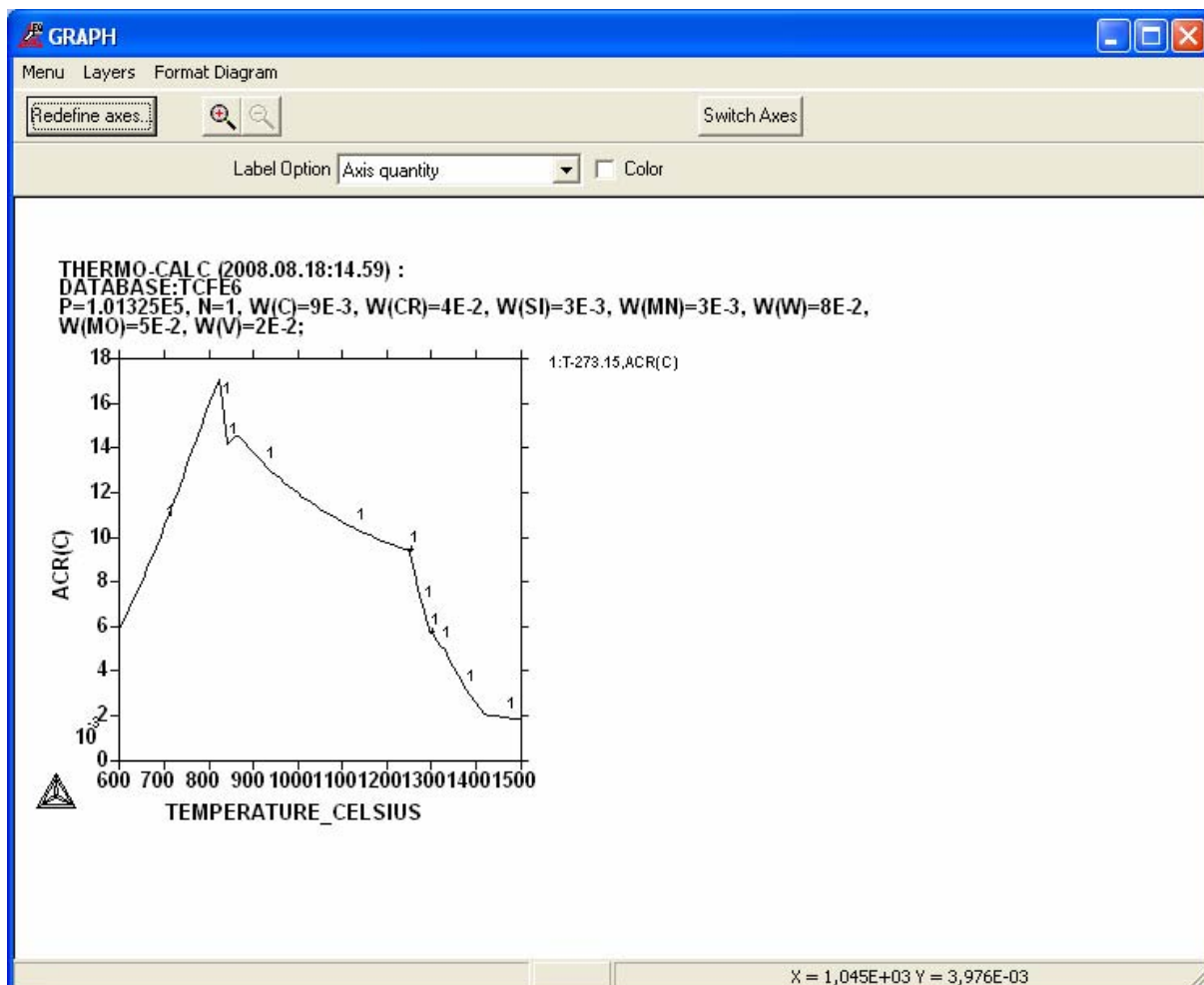
☐ SER Reference State

For Component: **C**

X-Axis Text: ☒ Automatic
TEMPERATURE_CELSIUS

Y-Axis Text: ☐ Automatic
ACR(C)

Back... ☐ New Graph Window Next Cancel Help



8. The magnitude of the carbon activity may seem strange in the last plot. This is because the default reference state for carbon is at room temperature in this database. Enter a function to refer the C activity to graphite at the temperature of the calculation. Click *Redefine* and open the *User Symbols* tab. Define the function ($ACT2=ACR(C,GRAPHITE)$) and move to *Advanced Diagram Axes* where you select the new function for the Y-axis. Click *Next* to plot.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | **Advanced Diagram Axes**

All Defined Symbols

ACT2=ACR(C,GRAPHITE)

Type: Function

Name:

Expression:

Add Symbol Delete Symbol Tabulate

X-Axis Text: ☒ Automatic
TEMPERATURE_CELSIUS

Y-Axis Text: ☐ Automatic
ACR(C)

Back... ☐ New Graph Window Next Cancel Help

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | **Advanced Diagram Axes**

Diagram Title:

X-Axis

Temperature and Pressure: Temperature Celsius

Potential and Activity:

Compositional Variables:

Phase Variables:

Energy Variables:

Additional Quantities:

Partial Derivatives:

User Symbols:

Y-Axis

Temperature and Pressure:

Potential and Activity:

Compositional Variables:

Phase Variables:

Energy Variables:

Additional Quantities:

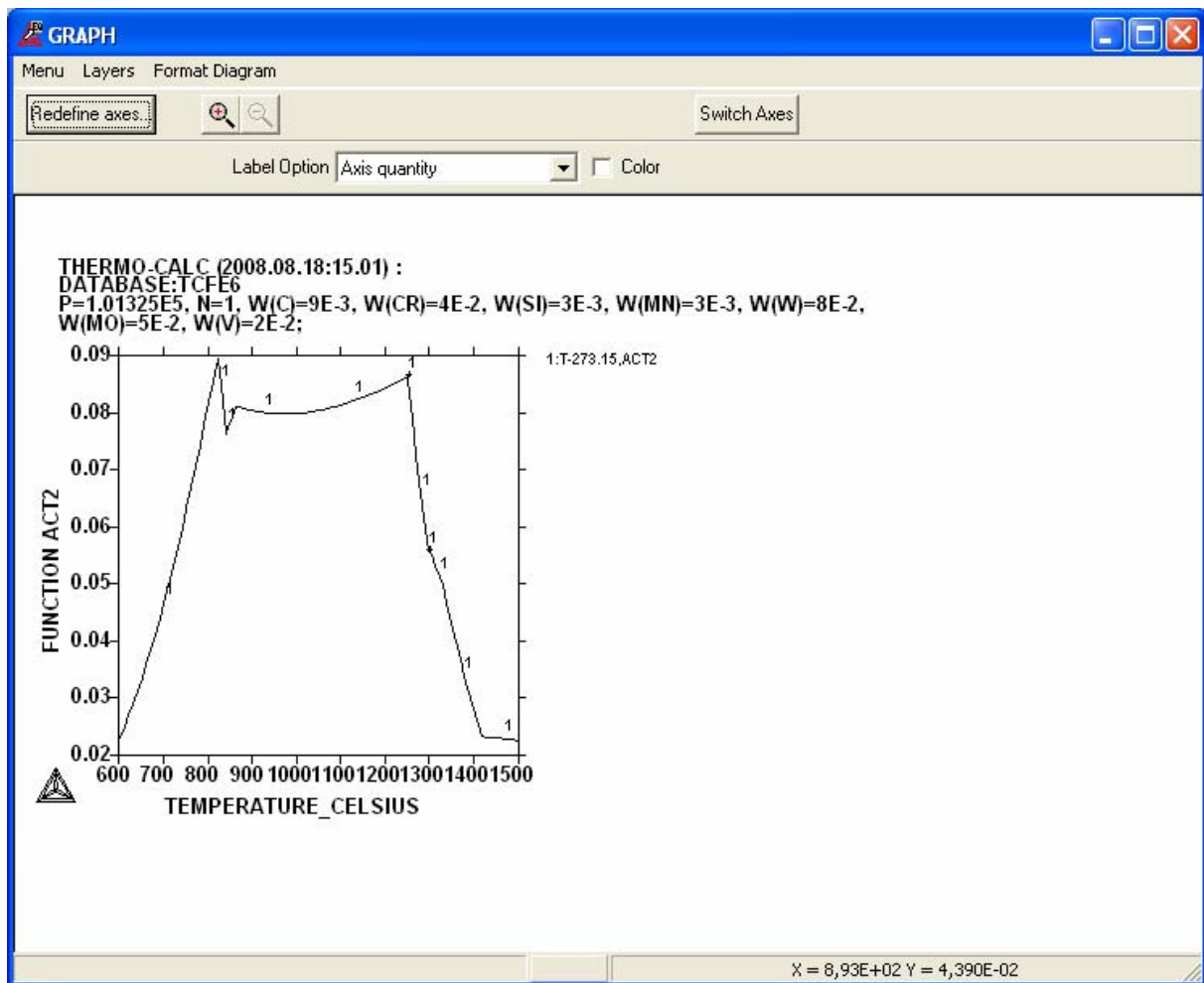
Partial Derivatives:

User Symbols: ACT2

X-Axis Text: ☒ Automatic
TEMPERATURE_CELSIUS

Y-Axis Text: ☐ Automatic
FUNCTION ACT2

Back... ☐ New Graph Window Next Cancel Help



9. Click *Redefine* to plot yet another property diagram, this time the composition of the M6C phase. Open the *Advanced Diagram Axes* tab and select *Phase Composition (moles)* for all components in the M6C phase as the Y-axis variable. Click *Next* to plot. In the diagram below, note that the M6C phase is stable for temperatures below 1304 °C and at larger temperatures the metastable composition is shown.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | Advanced Diagram Axes

Diagram Title

X-Axis

Temperature and Pressure: **Temperature Celsius** | Potential and Activity: |

Compositional Variables: | Phase Variables: |

Energy Variables: | Additional Quantities: |

Partial Derivatives: |

User Symbols: |

Y-Axis

Temperature and Pressure: | Potential and Activity: |

Compositional Variables: | Phase Variables: **Phase Composition (mC)** | For Component: **ALL** | For Phase: **M6C** |

Energy Variables: | Additional Quantities: |

Partial Derivatives: |

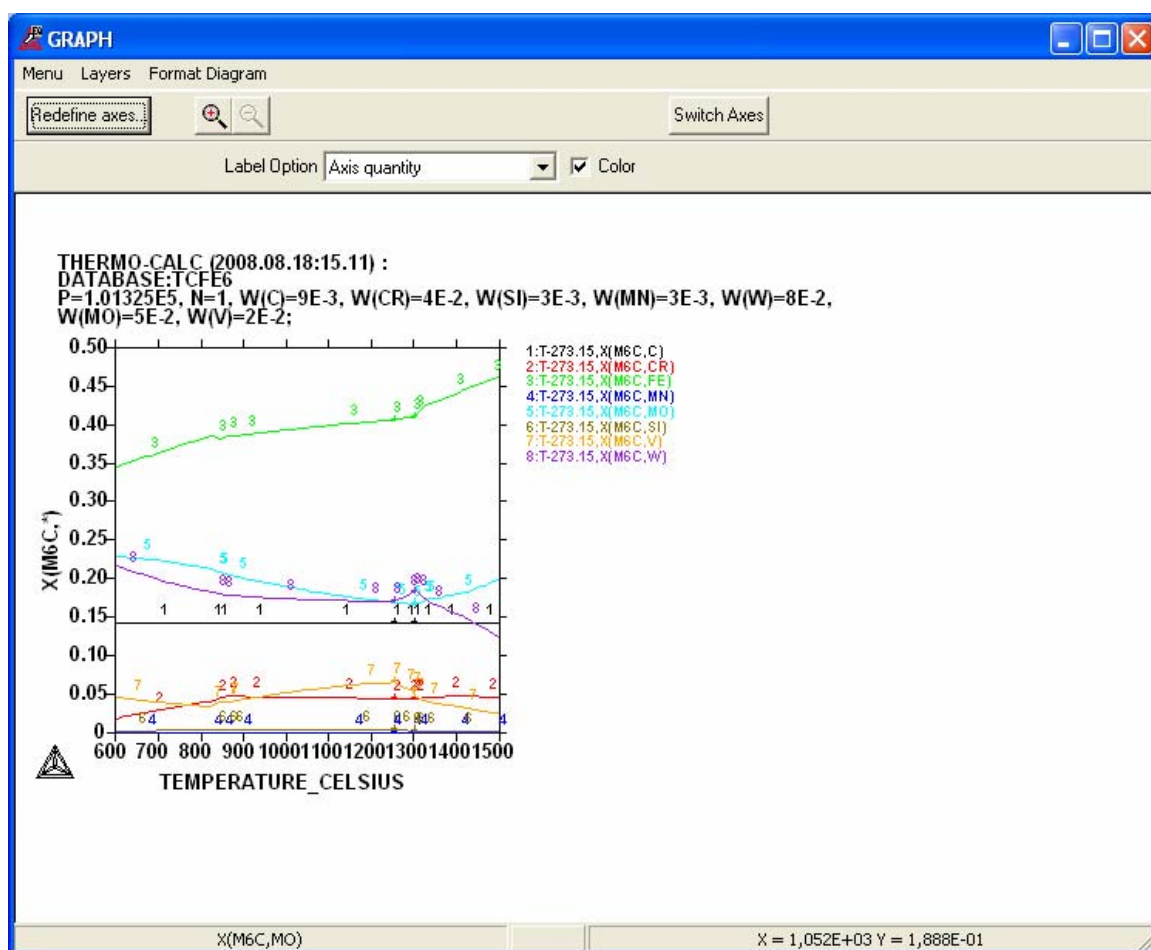
User Symbols: |

X-Axis Text: ☒ Automatic | **TEMPERATURE_CELSIUS**

Y-Axis Text: ☐ Automatic | **X(M6C,*)**

Back... ☐ New Graph Window Next Cancel Help

10. Select *Axis quantity* in the *Label Option* menu and check the color box.



8 Calculate Heat and Heat Capacity Variation during Solidification of an Al-15%Mg-9%Si Alloy

1. Click the *Elements* button in the MAIN window. Select database *PTERN* and elements *Al*, *Mg* and *Si* from the periodic table.
2. Click *Next* to come to the CONDITIONS window. Enter compositions in mass-fraction; 0.15 Mg and 0.09 Si, and the temperature 1000 K.

CONDITIONS

Number of Missing Conditions: 0

Temperature: 1000 K

Pressure: 101325 Pa

System Size: Moles 1 moles

Composition Unit: Mole-fraction

Component	Value	Condition
AL		Composition
MG	0.15	Composition
SI	9E-2	Composition

Redefine...

All Defined Conditions in SI Units:

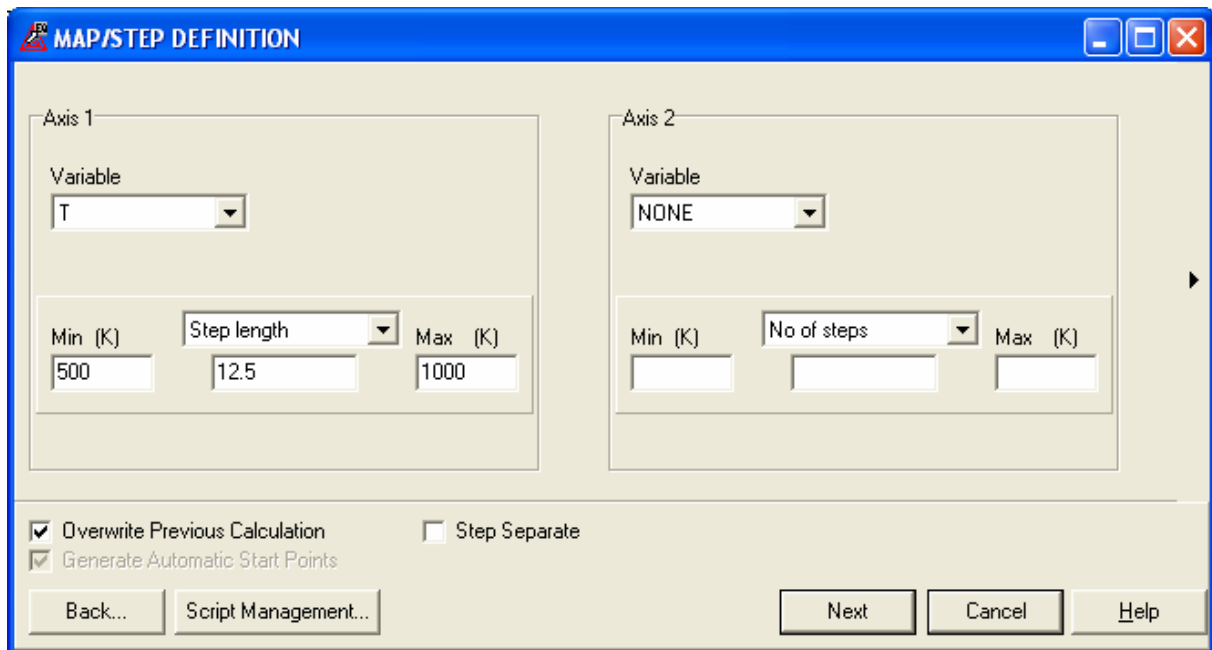
T=1000
P=1.01325E5
N=1
X(MG)=0.15
X(SI)=9E-2

Delete

Fixed Phases:

Back... Script Management... Show Value... Compute Next Cancel Help

3. Click next to open the MAP/STEP DEFINITION window. Set *T* as axis variable and step between 500 K and 1000 K with step length 12.5. Click *Next*.



MAP/STEP DEFINITION

Axis 1

Variable: T

Min (K): 500 Step length: 12.5 Max (K): 1000

Axis 2

Variable: NONE

Min (K): No of steps: Max (K):

☒ Overwrite Previous Calculation ☐ Step Separate

☒ Generate Automatic Start Points

Back... Script Management... Next Cancel Help

- Set diagram axis as *Temperature Kelvin* on X-axis and *Phase fraction* of all phases on Y-axis, default values. Click *Next* to plot. Choose *Stable phases* in the *Label Option* menu.

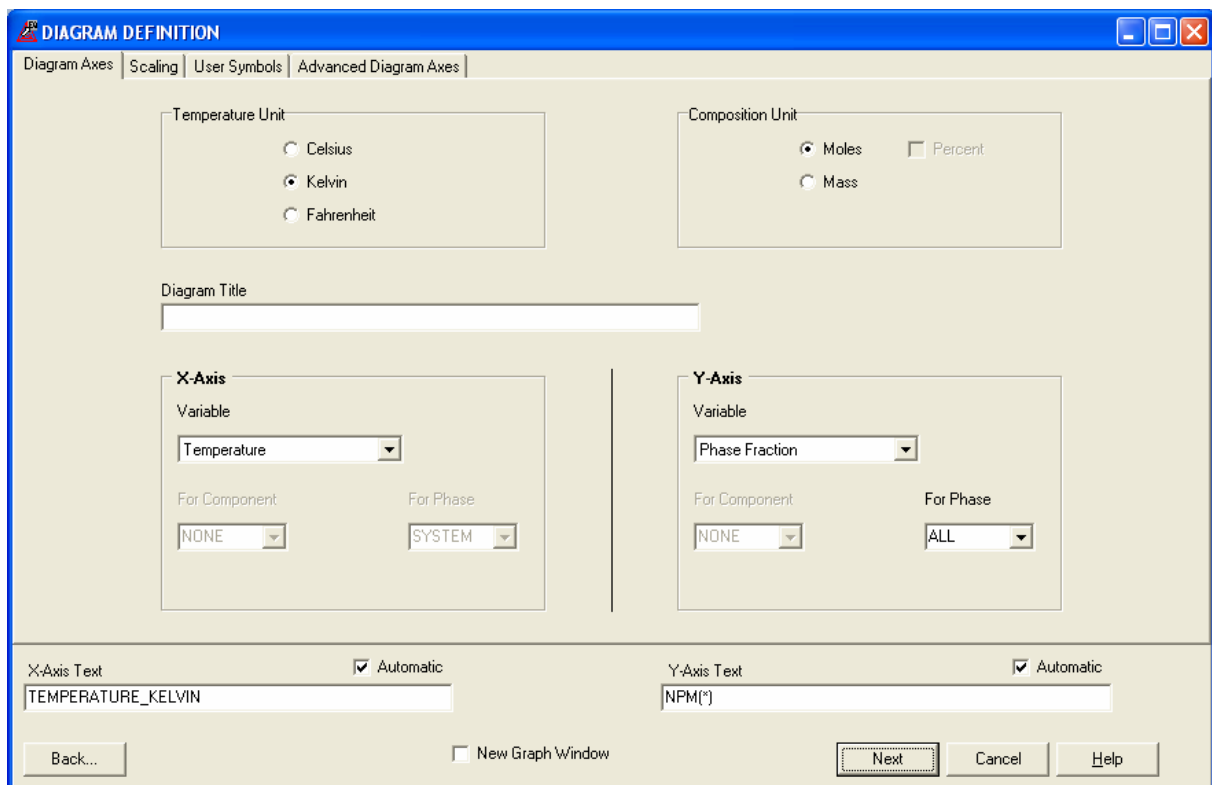


DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | Advanced Diagram Axes

Temperature Unit: ☐ Celsius ☒ Kelvin ☐ Fahrenheit

Composition Unit: ☒ Moles ☐ Percent ☐ Mass

Diagram Title:

X-Axis

Variable: Temperature

For Component: NONE For Phase: SYSTEM

Y-Axis

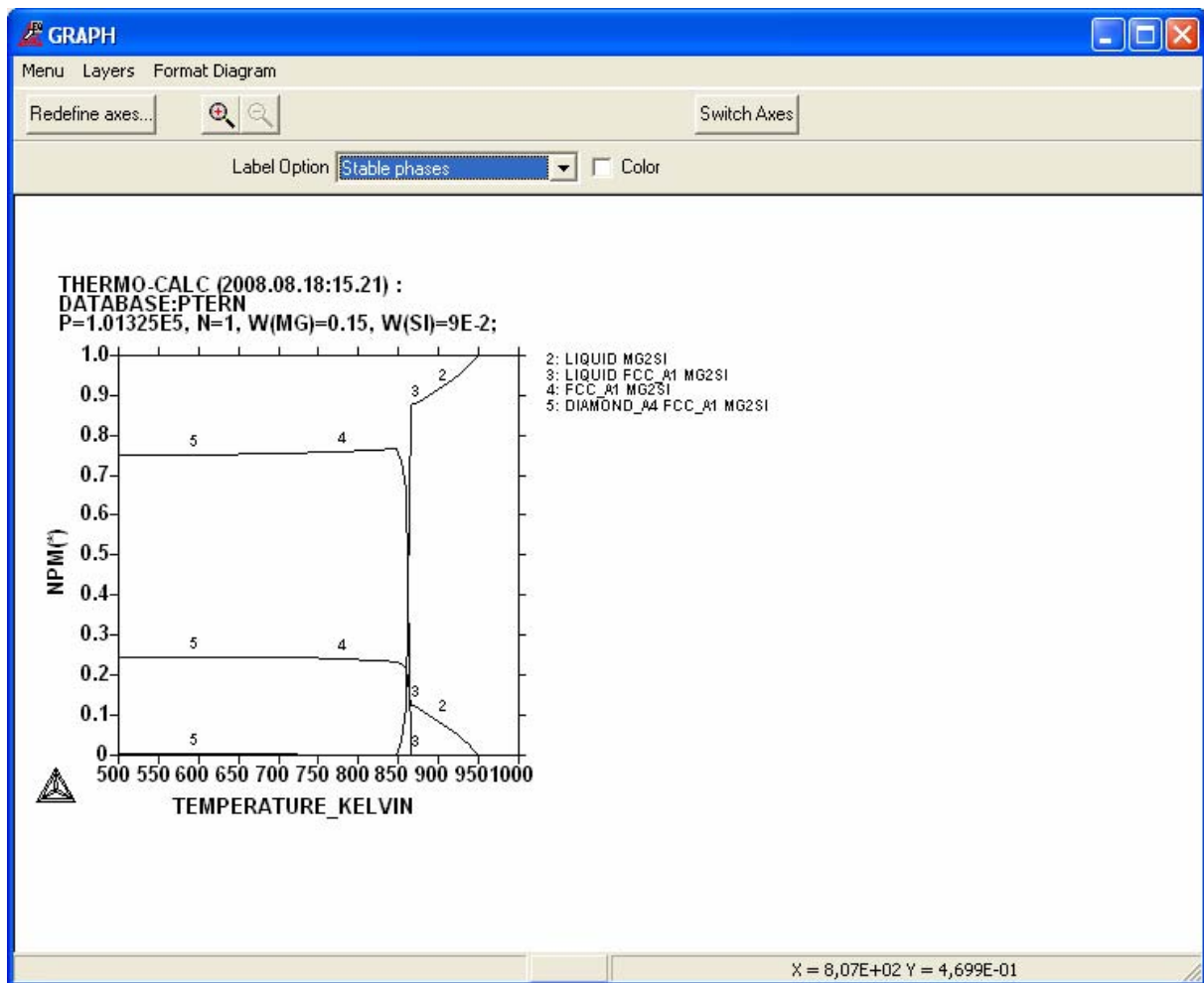
Variable: Phase Fraction

For Component: NONE For Phase: ALL

X-Axis Text: ☒ Automatic TEMPERATURE_KELVIN

Y-Axis Text: ☒ Automatic NPM[°]

Back... ☐ New Graph Window Next Cancel Help



- Now plot the total enthalpy (heat) as a function of temperature. Click *Redefine axes* in the GRAPH window to return to the DIAGRAM DEFINITION window. Open the *Advanced Diagram Axes* tab and select *Enthalpy normalized per mole* as variable on the Y-axis and select *SYSTEM*. Click *Next* to plot.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | Advanced Diagram Axes

Diagram Title

X-Axis

Temperature and Pressure: **Temperature Kelvin**

Potential and Activity:

Compositional Variables:

Phase Variables:

Energy Variables:

Additional Quantities:

Partial Derivatives:

User Symbols:

Y-Axis

Temperature and Pressure:

Potential and Activity:

Compositional Variables:

Phase Variables:

Energy Variables: **Enthalpy**

Additional Quantities:

Partial Derivatives:

User Symbols:

☐ SER Reference State

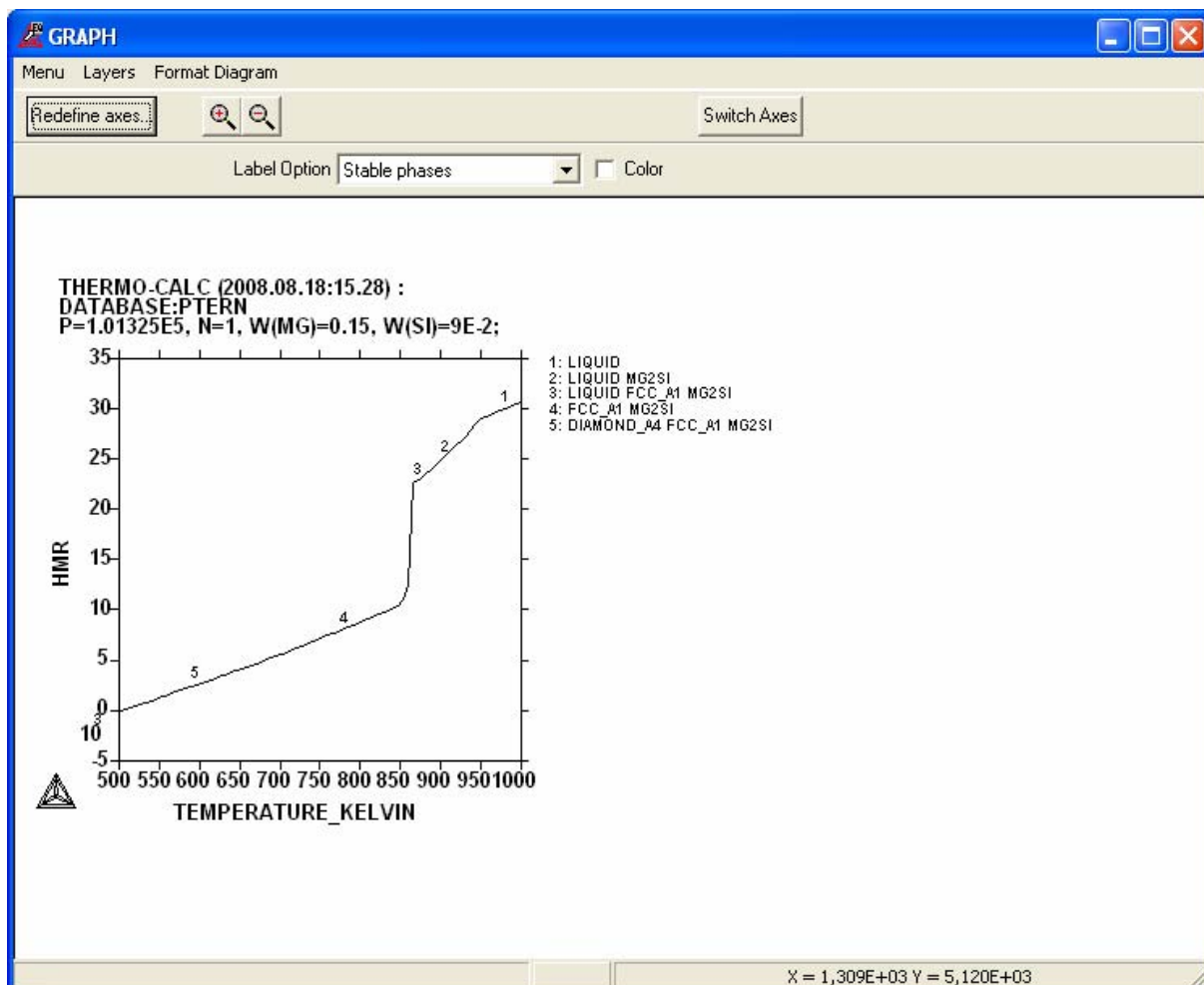
For Phase: **SYSTEM**

Normalization: **per mole**

X-Axis Text: ☒ Automatic
TEMPERATURE_KELVIN

Y-Axis Text: ☐ Automatic
HMR

Back... ☐ New Graph Window Next Cancel Help



- Next we want to plot the heat capacity. Click *Redefine axes* in the GRAPH window to return to the DIAGRAM DEFINITION window. Open the *Advanced Diagram Axes* tab and select *Heat capacity for system* as the Y-axis variable. Click *Next* to plot. Use the *zoom in* button to change the scaling of the plot.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | Advanced Diagram Axes

Diagram Title

X-Axis

Temperature and Pressure: **Temperature Kelvin** (selected)

Potential and Activity: (empty)

Compositional Variables: (empty)

Phase Variables: (empty)

Energy Variables: (empty)

Additional Quantities: (empty)

Partial Derivatives: (empty)

User Symbols: (empty)

Y-Axis

Temperature and Pressure: (empty)

Potential and Activity: (empty)

Compositional Variables: (empty)

Phase Variables: (empty)

Energy Variables: (empty)

Additional Quantities: (empty)

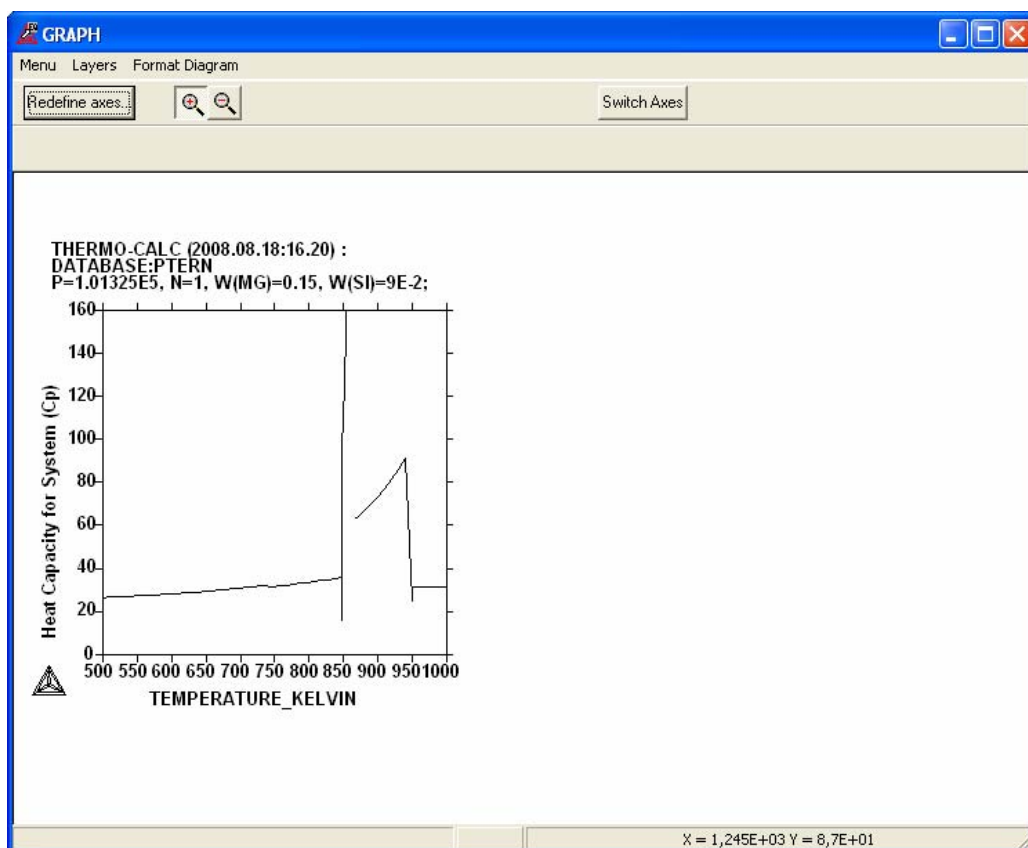
Partial Derivatives: **Heat capacity for system (HM.T)** (selected)

User Symbols: (empty)

X-Axis Text: ☒ Automatic
TEMPERATURE_KELVIN

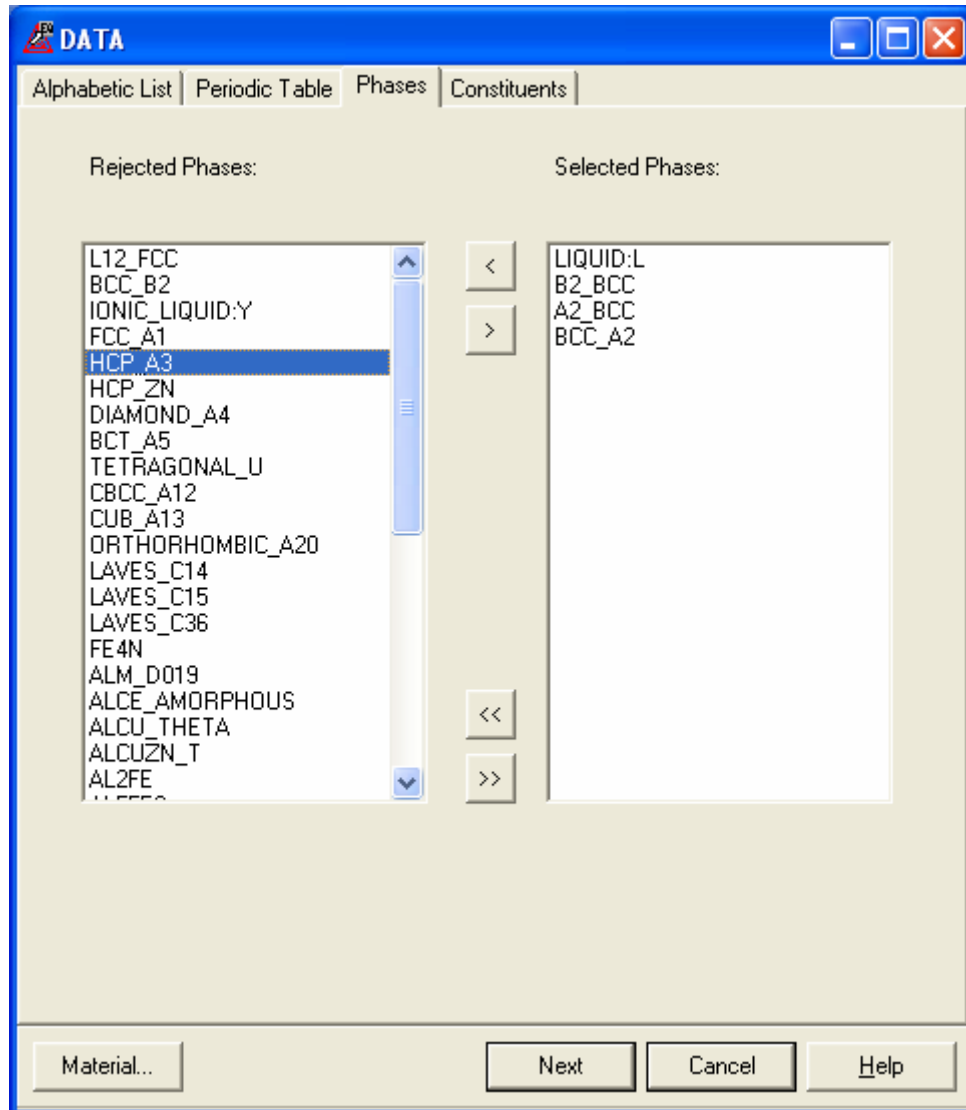
Y-Axis Text: ☐ Automatic
Heat Capacity for System (Cp)

Back... ☐ New Graph Window Next Cancel Help



9 Calculate Second Order Transition Line in Al-Fe System

1. Click the *Elements* button in the MAIN window and select database *SSOL4* and elements *Al* and *Fe* from the periodic table.
2. Reject all phases and select *LIQUID*, *B2_BCC*, *BCC_A2* and *A2_BCC* (disordered part of the *B2_BCC*).



3. Click *Next* to come to the CONDITIONS window. Select the composition unit mole-fraction and set the amount of Al to 0.4, and the temperature to 400 K.

CONDITIONS

Number of Missing Conditions: 1

Temperature: 400 K

Pressure: 101325 Pa

System Size: Moles 1 moles

All Defined Conditions in SI Units:

T=400
P=1.01325E5
N=1

Delete

Fixed Phases:

Set Reference State: Components

User Symbols: Advanced Conditions

Start Values: Phases





Composition Unit: Mole-fraction

Component	Value	Condition
AL	0.4	Composition
FE		Composition

Redefine...

Back... Script Management... Show Value... Compute Next Cancel Help

- To see how Al and Fe distribute on the sublattices click the *Options* in the MAIN window and select *Output*. Select *Constitution and Composition* and click *Ok*, then click *Compute*.

 **OUTPUT**   

☐ Save equilibrium output to file:

☒ Every output in new window

Fraction Order

☒ Value Order

☐ Alphabetical Order

Fraction Type

☒ Mass Fraction

☐ Mole Fraction

Composition Only?

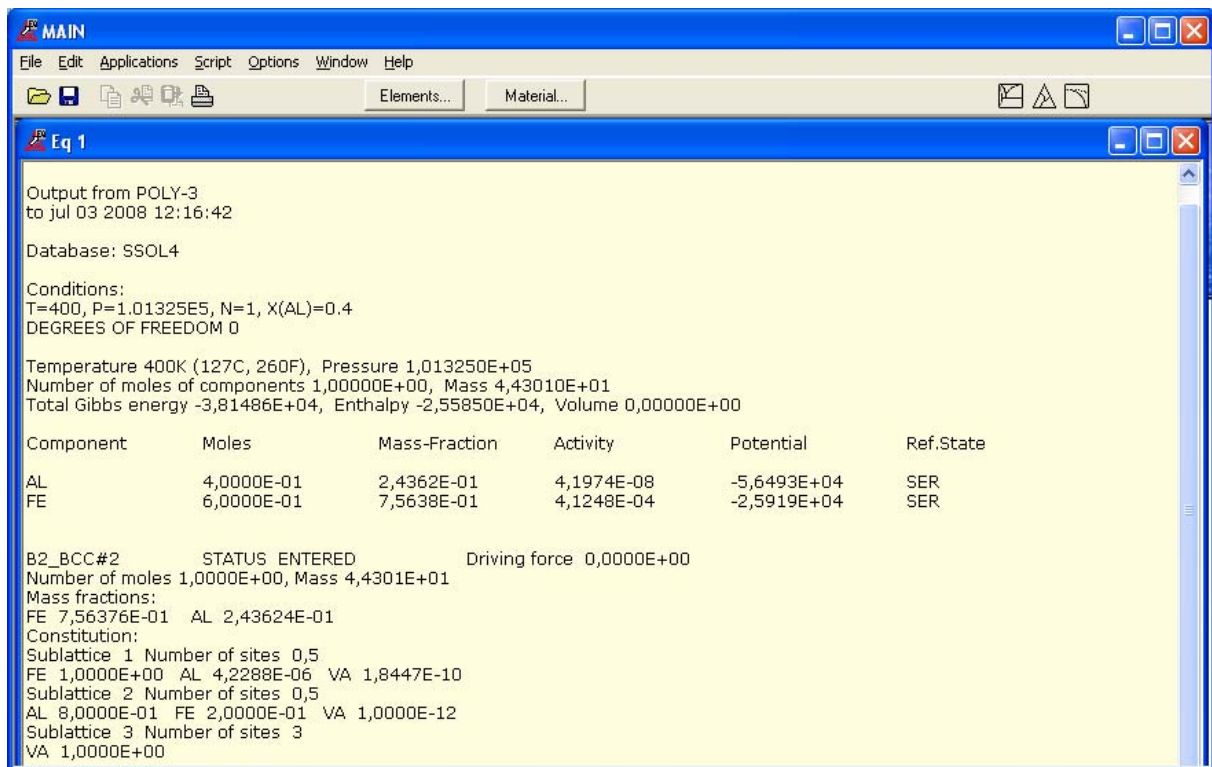
☐ Composition

☒ Constitution and Composition

Stable Phases Only?

☒ Stable Phases Only

☐ All Non-suspended Phases



5. Change the condition for the amount of Al to be that of a difference in site-fractions in the two sublattices. Remove the $X(AL)=0.4$ condition and enter $Y(B2_BCC\#2,FE\#1)-Y(B2_BCC\#2,FE\#2)=1E-2$ under the *Advanced Conditions* tab in the CONDITIONS window.
6. Click *Next* to open the MAP/STEP DEFINITION window. Set one axis variable to T with min and max values 400 K and 2000 K , and step length 10 . Then click *Next*.

MAP/STEP DEFINITION

Axis 1

Variable
T

Min (K) 400 Step length 10 Max (K) 2000

Axis 2

Variable
NONE

Min (K) No of steps Max (K)

☒ Overwrite Previous Calculation ☐ Step Separate
☒ Generate Automatic Start Points

Back... Script Management... Next Cancel Help

7. Select *Mole-Fraction of Fe* in *All* phases and *Temperature* as diagram axes. Click *Next* to plot.

DIAGRAM DEFINITION

Diagram Axes Scaling User Symbols Advanced Diagram Axes

Temperature Unit

☐ Celsius
☒ Kelvin
☐ Fahrenheit

Composition Unit

☒ Moles ☐ Percent
☐ Mass

Diagram Title

X-Axis

Variable
Composition

For Component FE For Phase ALL

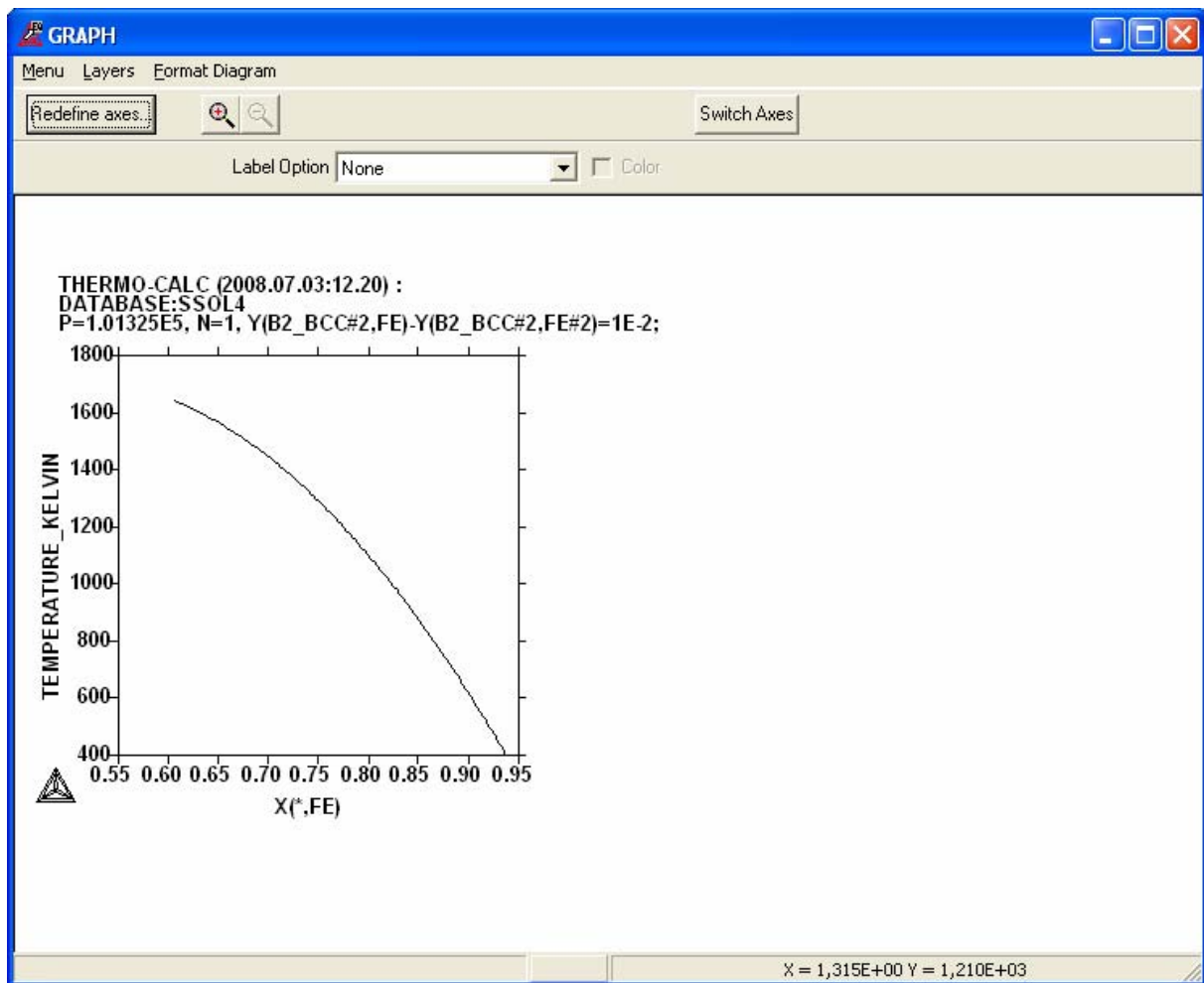
Y-Axis

Variable
Temperature

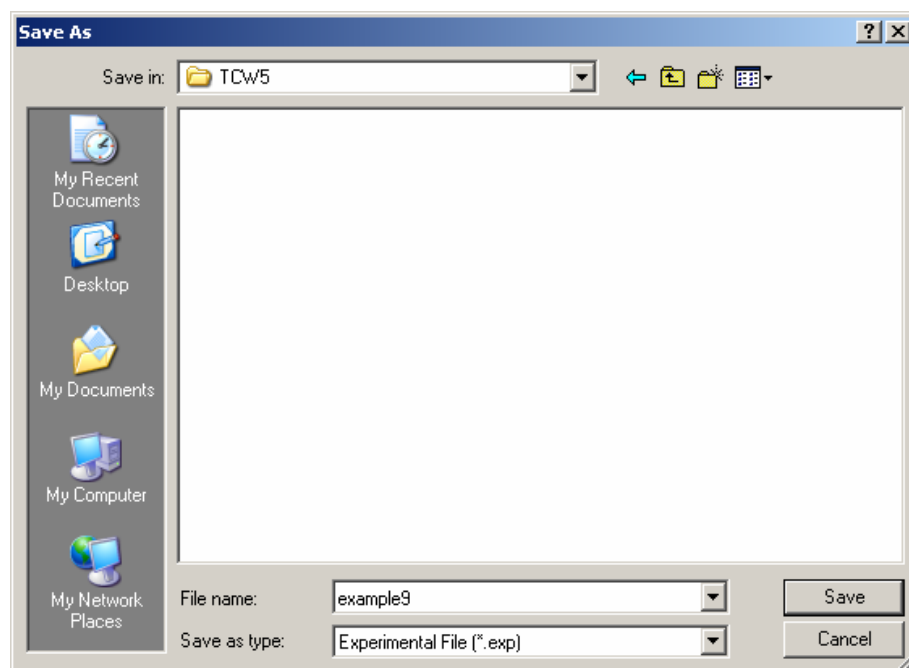
For Component NONE For Phase ALL

X-Axis Text ☒ Automatic [X(%.FE)] Y-Axis Text ☐ Automatic TEMPERATURE_KELVIN

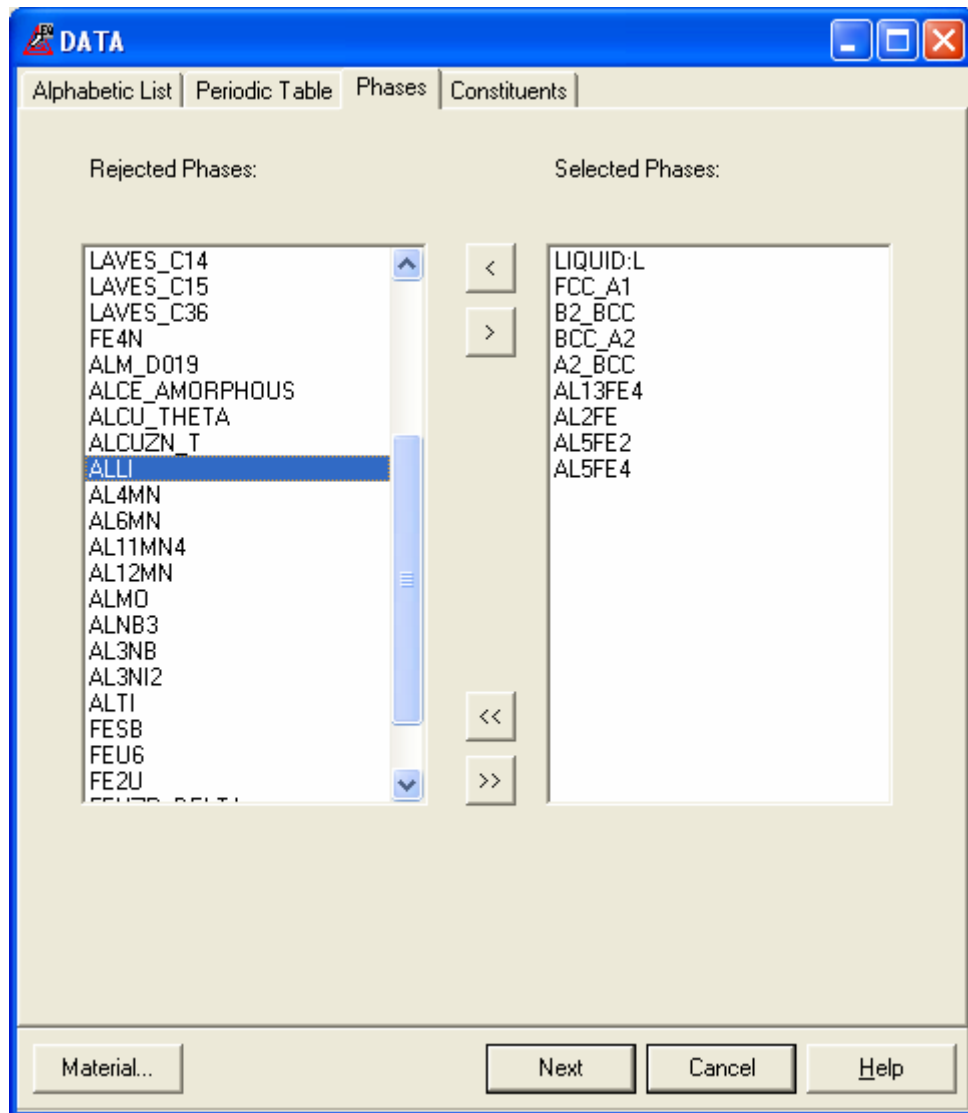
Back... ☐ New Graph Window Next Cancel Help



8. To plot the transition line in the Al-Fe phase diagram save the plot on an experimental file (e.g. example9.exp).



9. Close the GRAPH window and select *Elements* in the MAIN window. Reject all phases and select *LIQUID*, *FCC_A1*, *B2_BCC*, *BCC_A2*, *A2_BCC*, *AL13FE4*, *AL2FE*, *AL5FE2* and *AL5FE4*. Finally, click *Next*.



10. Enter $T=1300$ K and $X(\text{AL})=0.3$. Click *Next*.

CONDITIONS

Number of Missing Conditions: 0

Temperature: 1300 K

Pressure: 101325 Pa

System Size: Moles, 1 moles

All Defined Conditions in SI Units:

```
T=1300
P=1.01325E5
N=1
X(AL)=0.3
```

Delete

Fixed Phases:

Set Reference State: Components

User Symbols: Advanced Conditions

Start Values: Phases

Composition Unit: Mole-fraction

Component	Value	Condition
AL	0.3	Composition
FE		Composition

Redefine...

Back... Script Management... Show Value... Compute Next Cancel Help

11. Set X(AL) as axis variable for x-axis and T as axis variable for y-axis and click *Next* to map the phase diagram.

MAP/STEP DEFINITION

Axis 1:

Variable: X(AL)

Min: 0 No of steps: 50 Max: 1

Axis 2:

Variable: T

Min (K): 400 No of steps: 50 Max (K): 2273

☒ Overwrite Previous Calculation ☐ Step Separate

☒ Generate Automatic Start Points

Back... Script Management... Next Cancel Help

12. Select *Mole Fraction of Fe* and *Temperature* as diagram axes and click *Next* to plot.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | Advanced Diagram Axes

Temperature Unit
☐ Celsius
☒ Kelvin
☐ Fahrenheit

Composition Unit
☒ Moles ☐ Percent
☐ Mass

Diagram Title

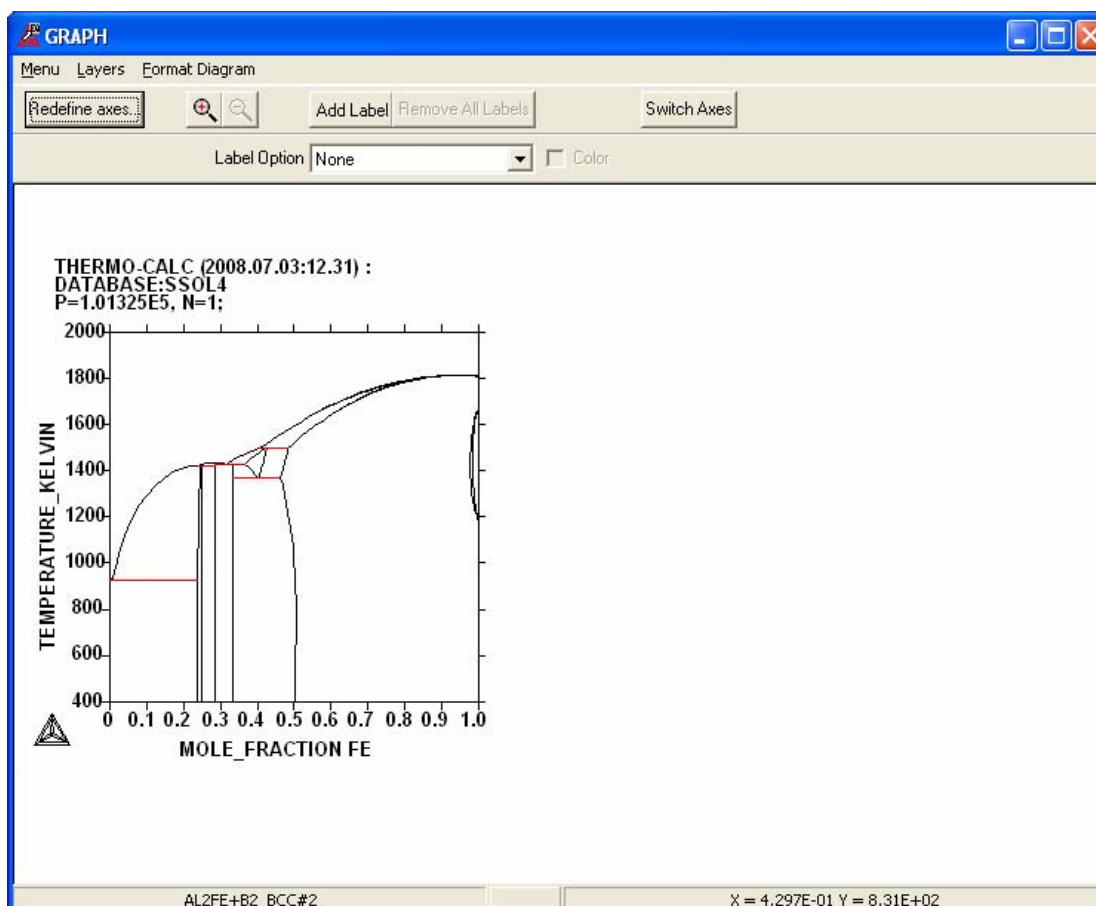
X-Axis
Variable
Composition
For Component: FE
For Phase: SYSTEM

Y-Axis
Variable
Temperature
For Component: NONE
For Phase: SYSTEM

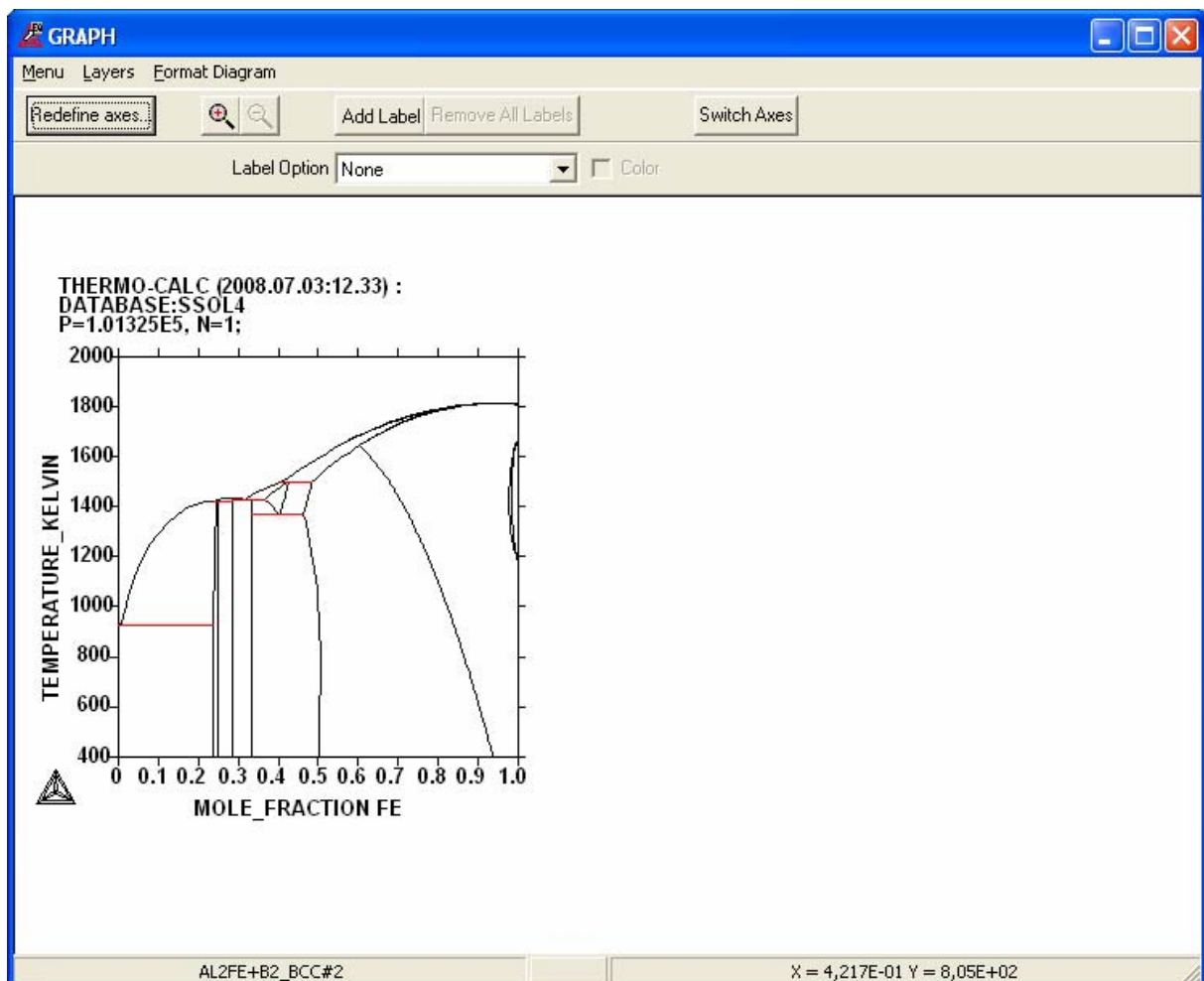
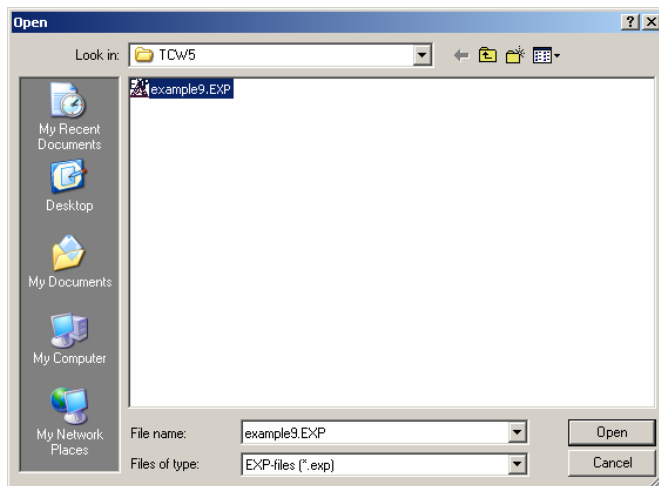
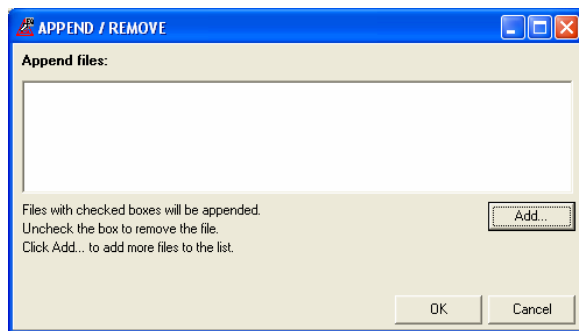
X-Axis Text ☒ Automatic
MOLE_FRACTION_FE

Y-Axis Text ☒ Automatic
TEMPERATURE_KELVIN

Back... ☐ New Graph Window Next Cancel Help

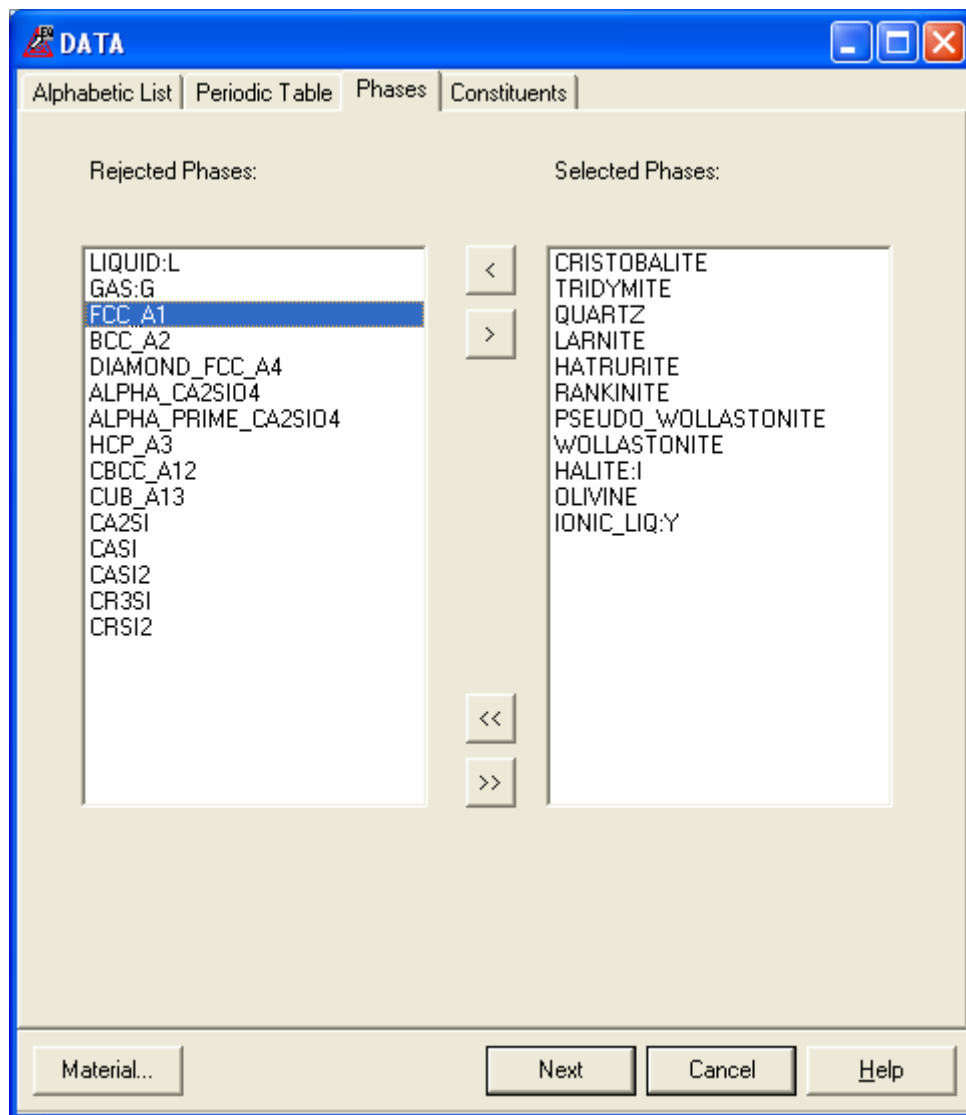


- To plot the transition line in the phase diagram select *Append* under *Menu* and find the experimental plot file created earlier (example9.EXP).

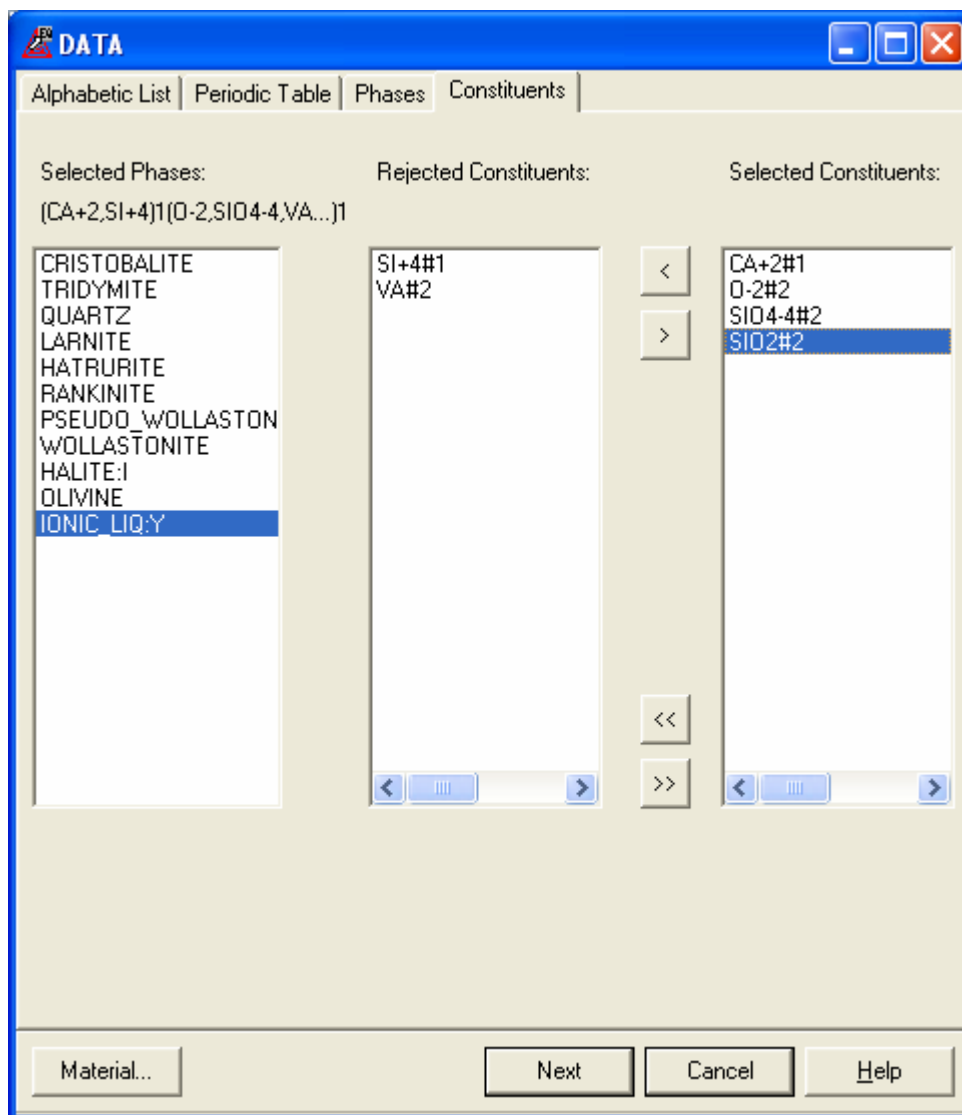


10 Calculate the CaO-SiO₂ System

1. Click the *Elements* button in the MAIN window.
2. Select database *PION* and elements *Ca*, *Si* and *O* from the periodic table.
3. Reject all phases and select only those we know should be stable in this system; CRISTOBALITE, TRIDYMITE, QUARTZ, LARNITE, HATRURITE, RANKINITE, PSEUDO_WOLLASTONITE, WOLLASTONITE, HALITE:I, OLIVINE, and IONIC_LIQ:Y.



4. Next, reject the following constituents from the IONIC_LIQ:Y phase: VA#2 and SI+4#1.



5. Click *Next* to come to the CONDITIONS window. Define more convenient components than the elements. Click *Redefine* and enter *CAO*, *SIO2* and *O*. Click *Ok* to return to the CONDITIONS window.
6. Enter temperature (2000 K), pressure (1E5 Pa) and size of the system (1 moles). Enter oxygen activity equal to one ($ACR(O)=1$) and mass-fraction *4E-1* for the SIO2 component.

CONDITIONS

Number of Missing Conditions: 0

Temperature: 2000 K

Pressure: 100000 Pa

System Size: Moles, 1 moles

All Defined Conditions in SI Units

T=2000
P=1E5
N=1
ACR(O)=1
X(SiO2)=0.4

Delete

Fixed Phases

Components

Set Reference State

Advanced Conditions

User Symbols

Phases

Start Values

Phase: IONIC_LIQ (CA+2)6(O-2,SiO4-4,SiO2)2

Amount: 0 moles

Major Constituent(s)

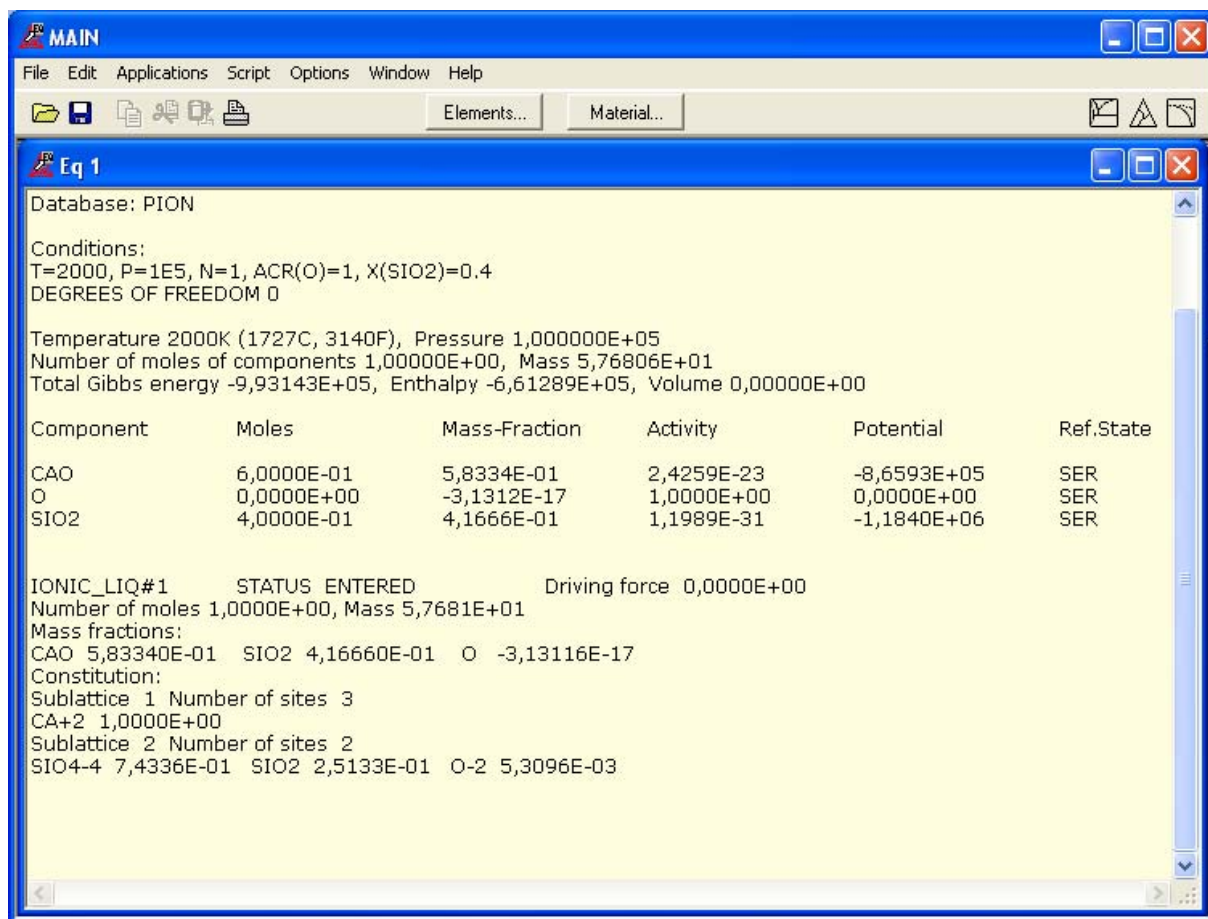
Sublattice	Major Constituents	Minor Constituents
Sublattice #1		
Sublattice #2	O-2	SiO4-4 SiO2

Force Start Values

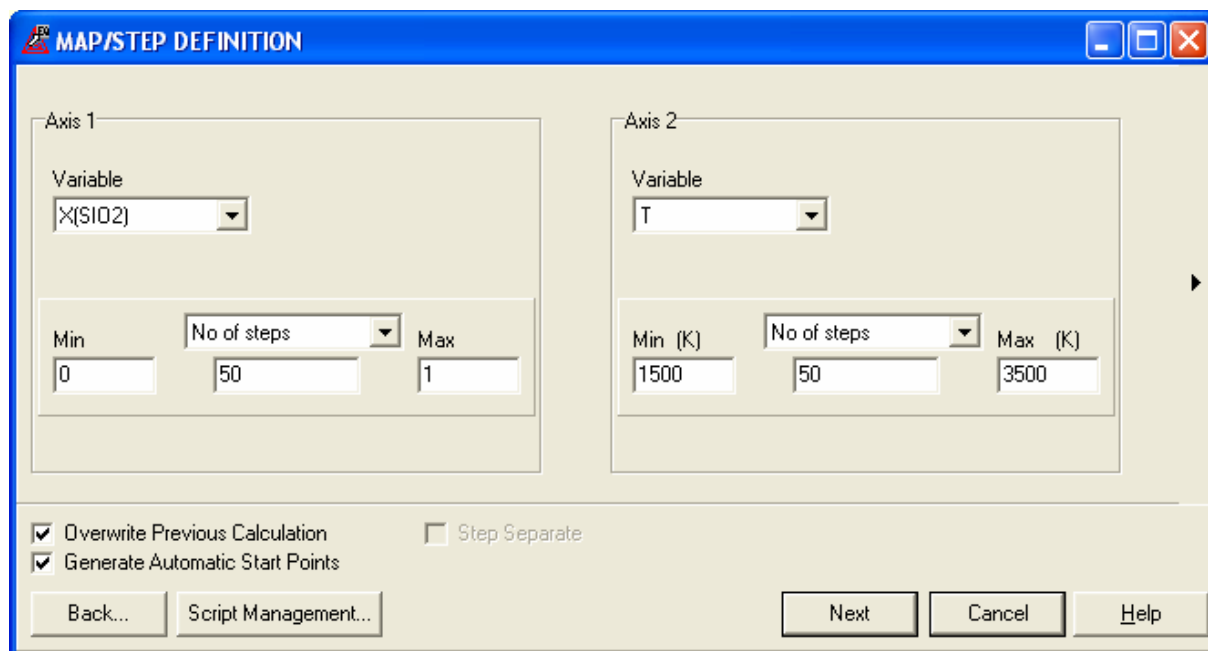
Phase Constituents...

Back... Script Management... Show Value... Compute Next Cancel Help

7. Click *Start Values* tab and change the major constituent in sublattice 2 in IONIC_LIQ to O-2.
8. Click *Compute* to perform an equilibrium calculation for the given conditions.

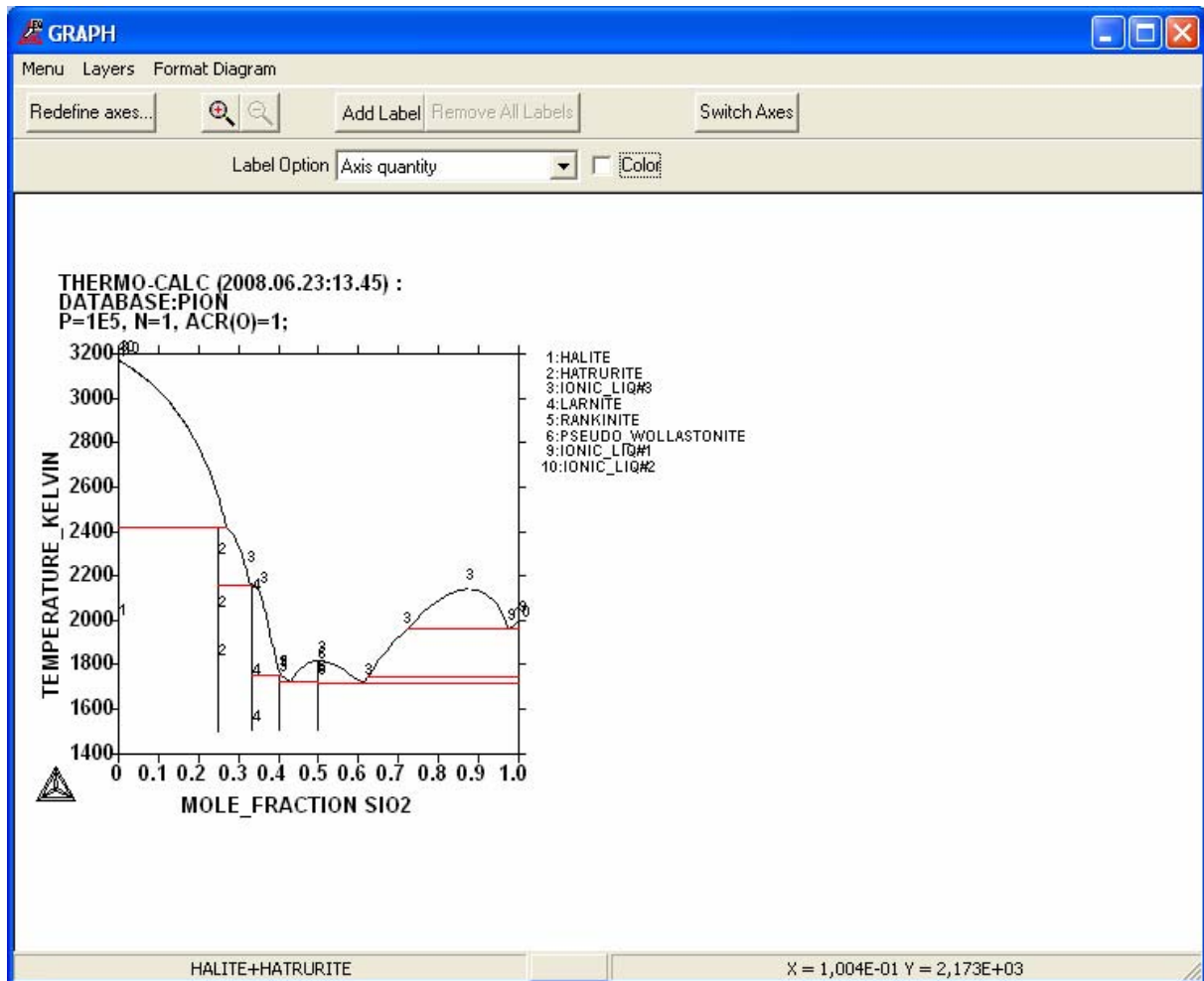


9. Click *Next* to come to the MAP/STEP DEFINITION window.
10. Select X(SIO2) and T as axis variable 1 and 2 respectively. Enter 0 and 1 as limits for axis 1 and 1500 and 3500, with step length 50, as limits for axis 2.



11. Click *Next* to execute the map command.

12. In the DIAGRAM DEFINITION window the suitable diagram axes should appear automatically (X(SiO₂) on x-axis and Temperature Kelvin on y-axis). Just click *Next* to plot and choose *Axis quantity* in the *Label Option* menu. .



11 Calculate A3 Temperature and Its Dependence on Alloying Element

1. Click the *Elements* button in the MAIN window.
2. Select database *TCFE6* and elements *C*, *Cr*, *Fe*, *Mn*, *Nb* and *Si* from the periodic table.
3. Click *Next* to come to the CONDITIONS window. Enter compositions in mass-fraction and the temperature: $W(\text{Cr})=1.5\text{E-}2$, $W(\text{C})=3\text{E-}3$, $W(\text{Mn})=5\text{E-}3$, $W(\text{Nb})=1\text{E-}3$, $W(\text{Si})=3\text{E-}3$, $T=1100\text{ K}$.

Number of Missing Conditions: 0

Temperature: 1100 K

Pressure: 101325 Pa

System Size: Moles 1 moles

All Defined Conditions in SI Units

```

T=1100
P=1.01325E5
N=1
W(C)=3E-3
W(MN)=5E-3
W(NB)=1E-3
W(SI)=3E-3
W(CR)=1.5E-2
    
```

Fixed Phases

Component	Value	Condition
C	3E-3	Composition
CR	1.5E-2	Composition
FE		Composition
MN	5E-3	Composition
NB	1E-3	Composition
SI	3E-3	Composition

Buttons: Back... Script Management... Show Value... Compute Next Cancel Help

4. Click *Compute* to perform an equilibrium calculation for the given conditions.
5. Fix the BCC_A2 phase with zero moles and remove the temperature condition.

CONDITIONS

Degrees of freedom: -1

Temperature: 1100 K

Pressure: 101325 Pa

System Size: Moles 1 moles

All Defined Conditions in SI Units:

```

T=1100
P=1.01325E5
N=1
W(C)=3E-3
W(MN)=5E-3
W(NB)=1E-3
W(SI)=3E-3
W(CR)=1.5E-2

```

Delete

Fixed Phases:

```

BCC_A2 = 0.00

```

Set Reference State | User Symbols | Start Values

Components | Advanced Conditions | Phases

Phases	Status	Moles
LIQUID	ENTERED	1.00
AL4C3	ENTERED	0.00
BCC_A2	FIXED	0.00
CEMENTITE	ENTERED	0.00
CHI_A12	ENTERED	0.00
CR3SI	ENTERED	0.00
DIAMOND_FCC_A4	ENTERED	0.00
FCC_A1	ENTERED	1.00
FCC_A1#2	ENTERED	0.00
FE2SI	ENTERED	0.00
FE4N_LP1	ENTERED	0.00
FE8SI2C	ENTERED	0.00
FECN_CHI	ENTERED	0.00
GRAPHITE	ENTERED	0.00

Phase Status:

FIXED 0.00 moles

Phase Conditions...

Add Composition Set...

Back... Script Management... Show Value... Compute Next Cancel Help

- Click *Compute* once more.
- To get the A_3 temperature click *Show Value* button and choose *Temperature Kelvin* in the SHOW VALUE window. Click *Show* to see the value.

CONDITIONS

Number of Missing Conditions:

Temperature: K

Pressure: Pa

System Size: moles

All Defined Conditions in SI Units

```
P=1.01325E5
N=1
W(C)=3E-3
W(MN)=5E-3
W(NB)=1E-3
W(SI)=3E-3
W(CR)=1.5E-2
```

Delete

Fixed Phases

```
BCC_A2 = 0.00
```

Set Reference State | User Symbols | Start Values

Components | Advanced Conditions | Phases

Composition Unit:

Component	Value	Condition
C	3E-3	Composition
CR	1.5E-2	Composition
FE		Composition
MN	5E-3	Composition
NB	1E-3	Composition
SI	3E-3	Composition

Redefine...

Back... Script Management... Show Value... Compute Next Cancel Help

SHOW VALUE

Temperature and Pressure:

Potential and Activity:

Compositional Variables:

Phase Variables:

Energy Variables:

Additional Quantities:

Partial Derivatives:

User Symbols:

Show

Show Value of:

Variable	Mnemonic	Value
Temperature (Kelvin)	T-K	1071.61

☒ Calculate Equilibrium Clear Close

- To investigate the dependence of the A_3 temperature on alloy composition, try changing one of the mass-fractions and click *Compute* after each change. Click *Show* in the SHOW VALUE window to see the new temperature.

12 Mapping of Univariant Equilibria of Liquid in the Fe-C-Cr System

1. Click *Elements* in the MAIN window.
2. Select *PTERN* from the *Database* list and then click alloy elements *Fe*, *C*, and *Cr* in the periodic table. Click *Next*.
3. Specify the concentrations of C and Cr as 1 and 5 *mass-percent*, respectively and change the temperature to 2000 K. Click *Next*.

CONDITIONS

Number of Missing Conditions: 0

Temperature: 2000 K

Pressure: 101325 Pa

System Size: Moles 1 moles

All Defined Conditions in SI Units

```
T=1000
P=1.01325E5
N=1
W(C)=1E-2
W(CR)=5E-2
```

Delete

Fixed Phases

Component	Value	Condition
FE		Composition
C	1	Composition
CR	5	Composition

Composition Unit: Mass-percent

Back... Script Management... Show Value... Compute Next Cancel Help

4. Set the variable for *Axis 1* to $W(C)$ and the variable for *Axis 2* to $W(CR)$. Click the arrow on the right of the window, and the panel for *Axis 3* appears. Choose T as the variable for the third axis and select *LIQUID* as the *Present Phase* since we are going to map the univariant equilibrium lines for the liquid phase. Click *Next*.

MAP/STEP DEFINITION

Axis 2

Variable:

Min (%): No of steps: Max (%):

Axis 3

Variable: Set Present Phase:

Min (K): No of steps: Max (K):

☒ Overwrite Previous Calculation ☐ Step Separate
☒ Generate Automatic Start Points

5. The default axes are mass-fraction of C and CR in the LIQUID phase. Accept this choice and click *Next*.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | Advanced Diagram Axes

Temperature Unit

☐ Celsius
☐ Kelvin
☐ Fahrenheit

Composition Unit

☐ Moles ☐ Percent
☒ Mass

Diagram Title:

X-Axis

Variable:

For Component: For Phase:

Y-Axis

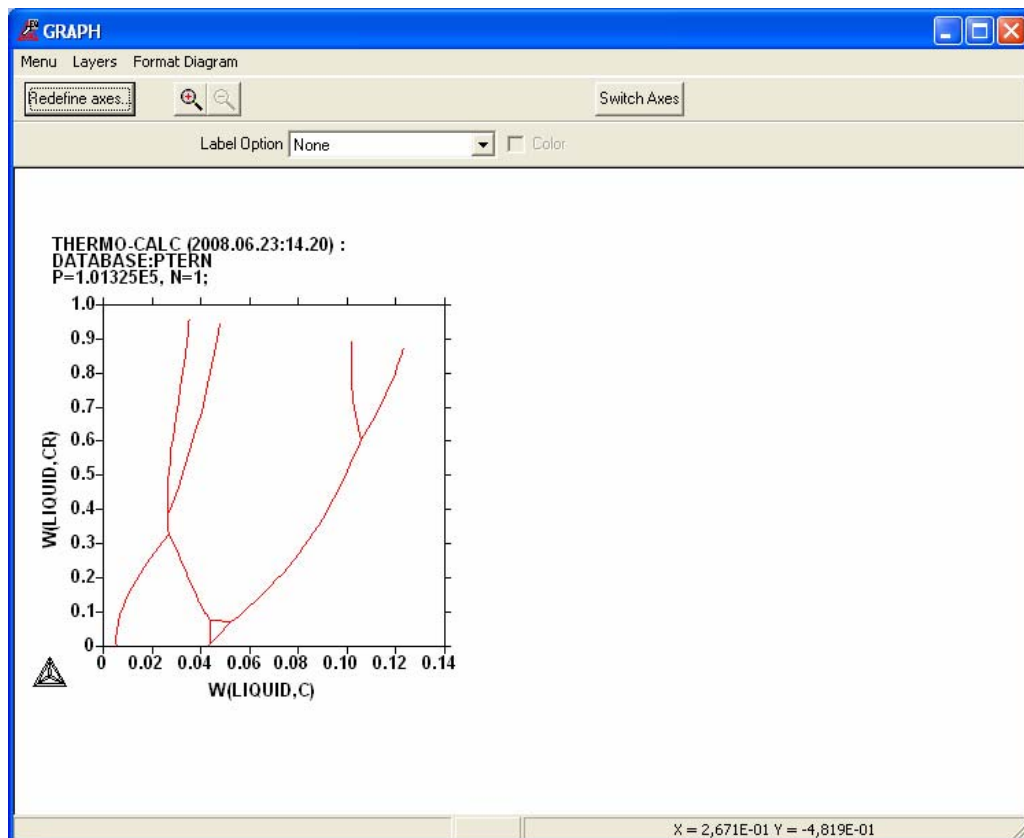
Variable:

For Component: For Phase:

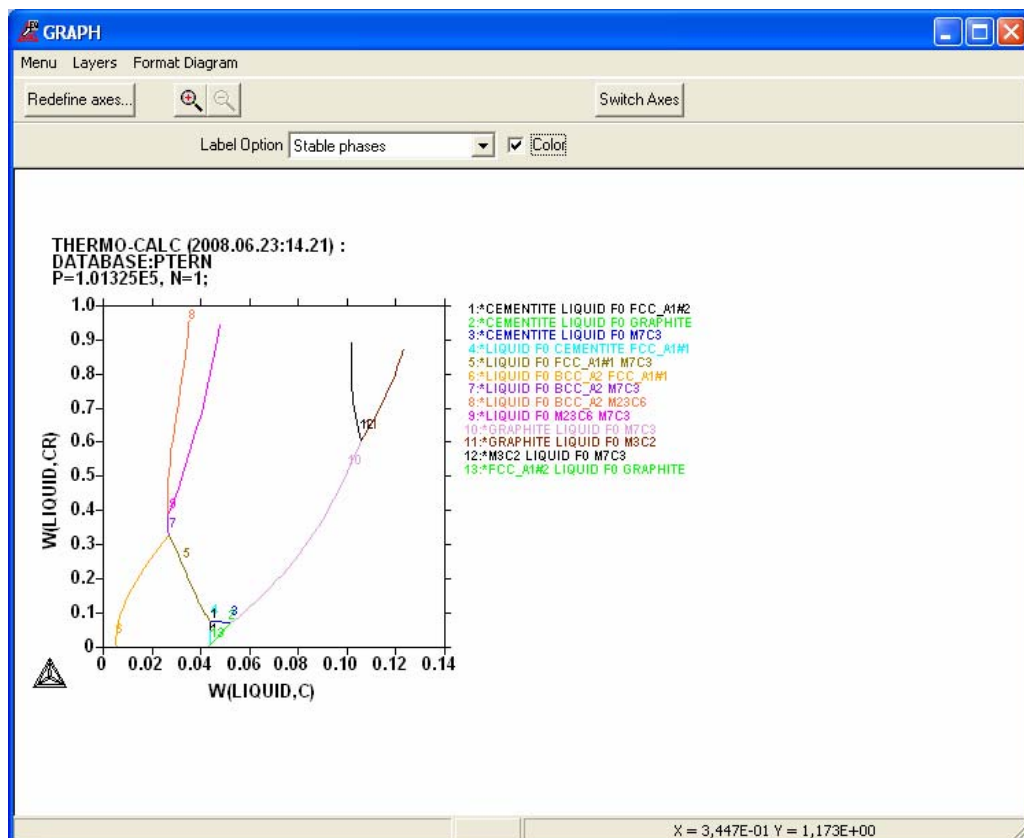
X-Axis Text: ☒ Automatic
 Y-Axis Text: ☒ Automatic

☐ New Graph Window

6. The univariant lines of the liquid phase are plotted.



- To identify the regions of different primary phases, choose *Stable phases* in the *Label option* menu and check the color box.



13 Plotting of Partial Pressure of Gas Species Along Solubility Lines in As-Ga Phase Diagram

1. Click Elements in the MAIN window. Select database *PG35* and elements *As* and *Ga* in the periodic system.
2. Reject all phases and select phases *LIQUID*, *RHOMBO_A7*, *ORTHO*, *FCC_B3* and *GAS*. Click *Next*.
3. Enter the conditions $T=1200$ K and $X(\text{GA})=0.3$. Put the *GAS* phase as *DORMANT*, which means that the phase is not considered in the equilibrium calculation but the driving force is calculated.

CONDITIONS

Number of Missing Conditions: 0

Temperature: 1200 K

Pressure: 101325 Pa

System Size: Moles, 1 moles

All Defined Conditions in SI Units:

T=1200
P=1.01325E5
N=1
X(GA)=0.3

Delete

Fixed Phases:

Phases	Status	Moles
GAS	DORMANT	0.00
FCC_B3	ENTERED	0.00
LIQUID	ENTERED	0.00
ORTHO	ENTERED	0.00
RHOMBO_A7	ENTERED	0.00

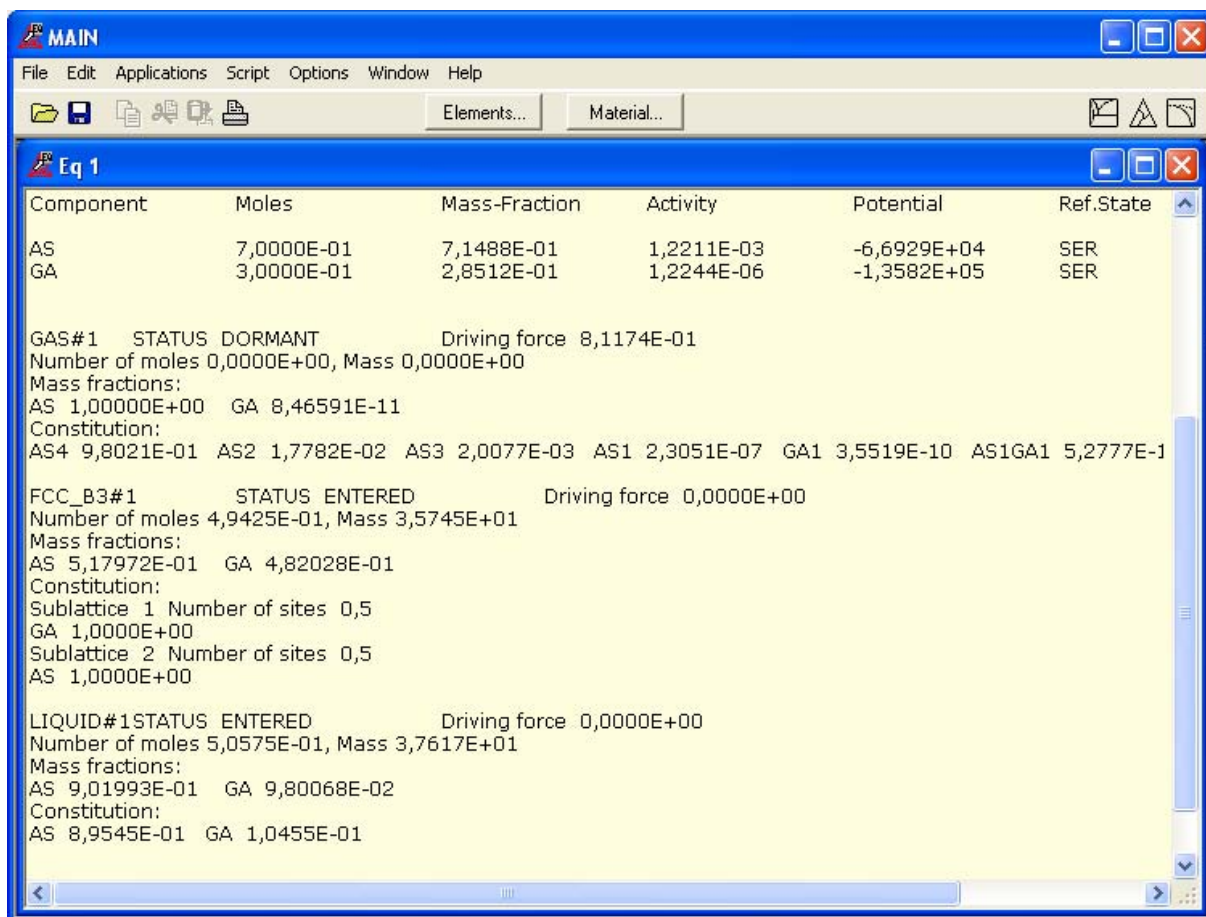
Phase Status: DORMANT moles

Phase Conditions...

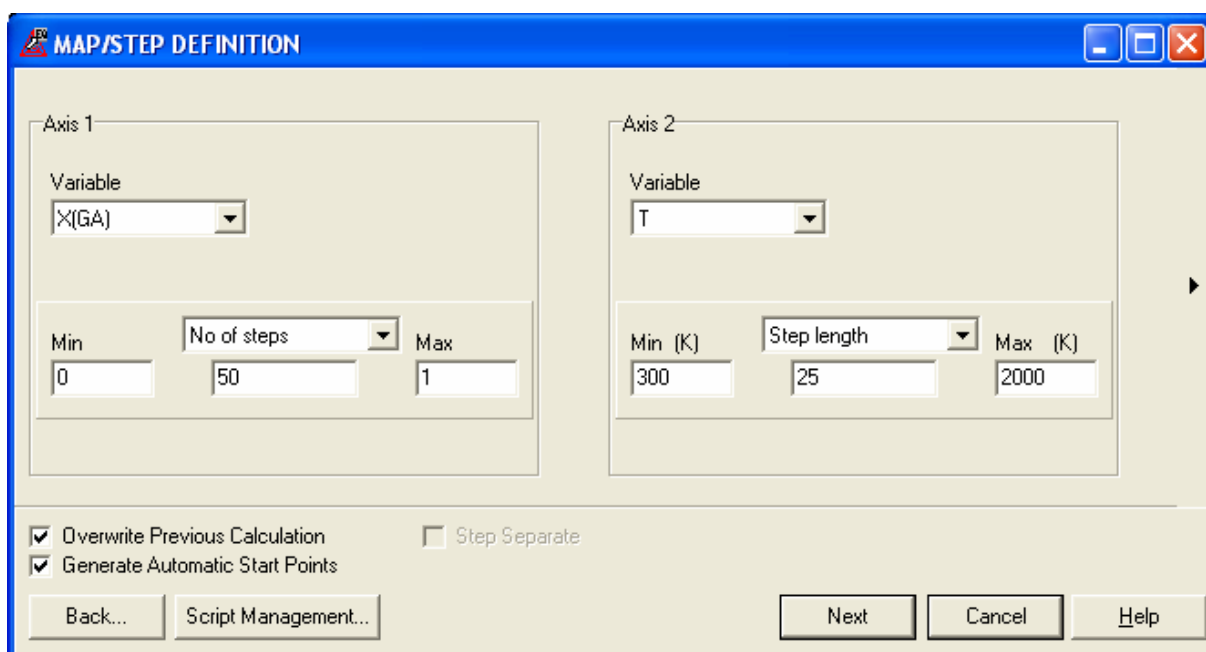
Add Composition Set...

Back... Script Management... Show Value... Compute Next Cancel Help

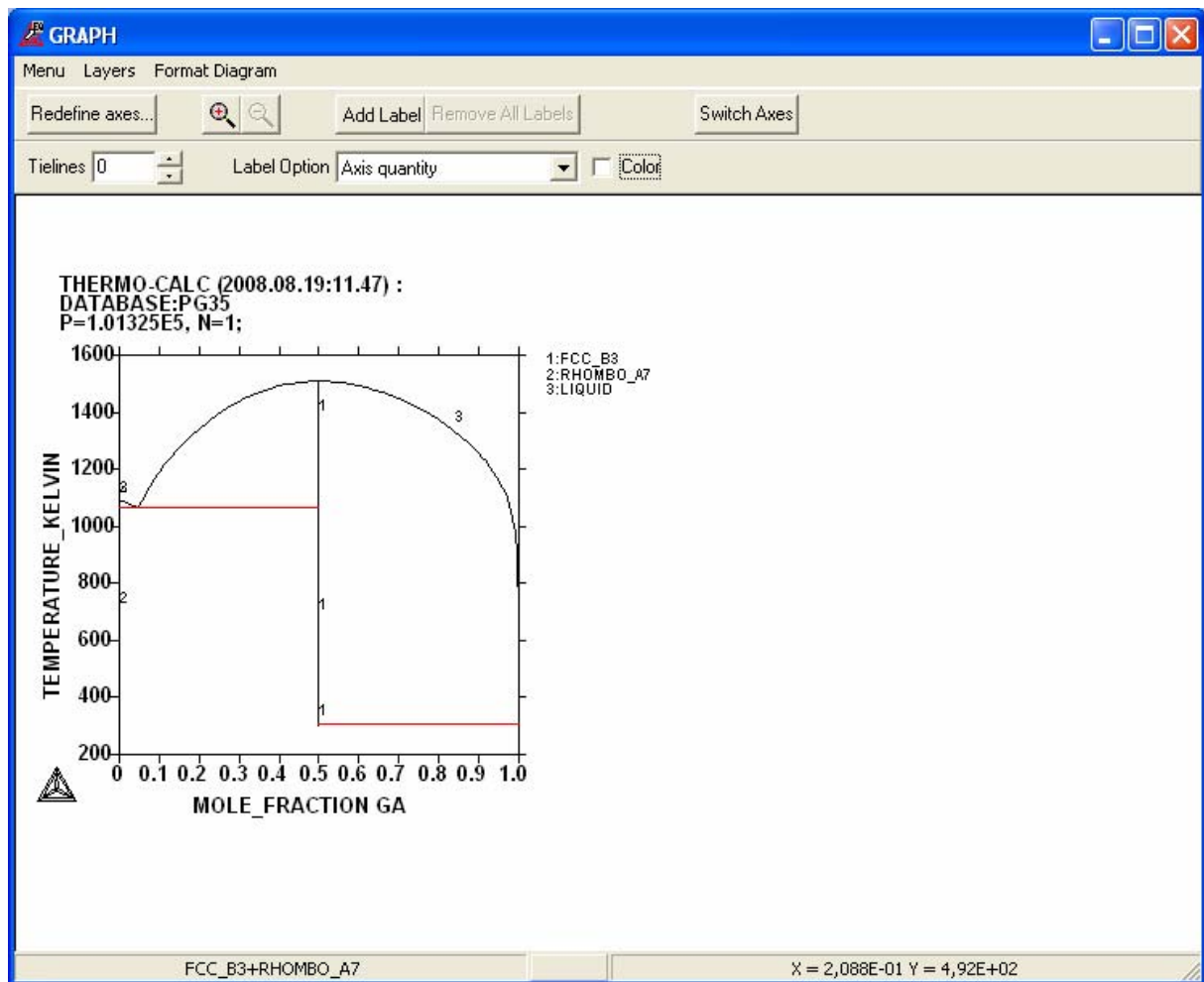
4. Click *Compute*.
5. From the equilibrium calculation it can be seen that the GAS phase would like to be stable (positive driving force) but it is not allowed to form as it is dormant. Click *Next*.



- To map the phase diagram set $X(\text{GA})$ with range 0 to 1 and T with range 300 to 2000 (step length 25) as axis variables. Click *Next* to map.



- Accept the default diagram axes. Click *Next* to plot the As-Ga phase diagram.



8. Now, one may be interested to know the partial pressures of the different gas species along the solubility lines. Click *Redefine* to return to the DIAGRAM DEFINITION window. Click the *User Symbols* tab and enter a number of functions and collect these in a table (see below).

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | **Advanced Diagram Axes**

All Defined Symbols

```
PAS3= 4343*LNACR(AS3,GAS)
PAS1= 4343*LNACR(AS1,GAS)
PAS2= 4343*LNACR(AS2,GAS)
PAS4= 4343*LNACR(AS4,GAS)
PASGA= 4343*LNACR(AS1GA1,GAS)
PGA1= 4343*LNACR(GA1,GAS)
IT=1000/T
PP=PAS1,PAS2,PAS3,PAS4,PASGA,PGA1
```

Type: **Table** Name:

Expression:

Add Symbol **Delete Symbol** **Tabulate**

X-Axis Text: ☒ Automatic Y-Axis Text: ☒ Automatic

Back... ☐ New Graph Window **Next** **Cancel** **Help**

- Go to the *Advanced Diagram Axes* tab and set *IT* on the X-axis and table *PP* on the Y-axis. Click *Next* to plot. In the GRAPH window select *Axis quantity* in the *Label Option* menu.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | **Advanced Diagram Axes**

Diagram Title:

X-Axis

Temperature and Pressure: Potential and Activity:

Compositional Variables: Phase Variables:

Energy Variables: Additional Quantities:

Partial Derivatives:

User Symbols: **IT**

Y-Axis

Temperature and Pressure: Potential and Activity:

Compositional Variables: Phase Variables:

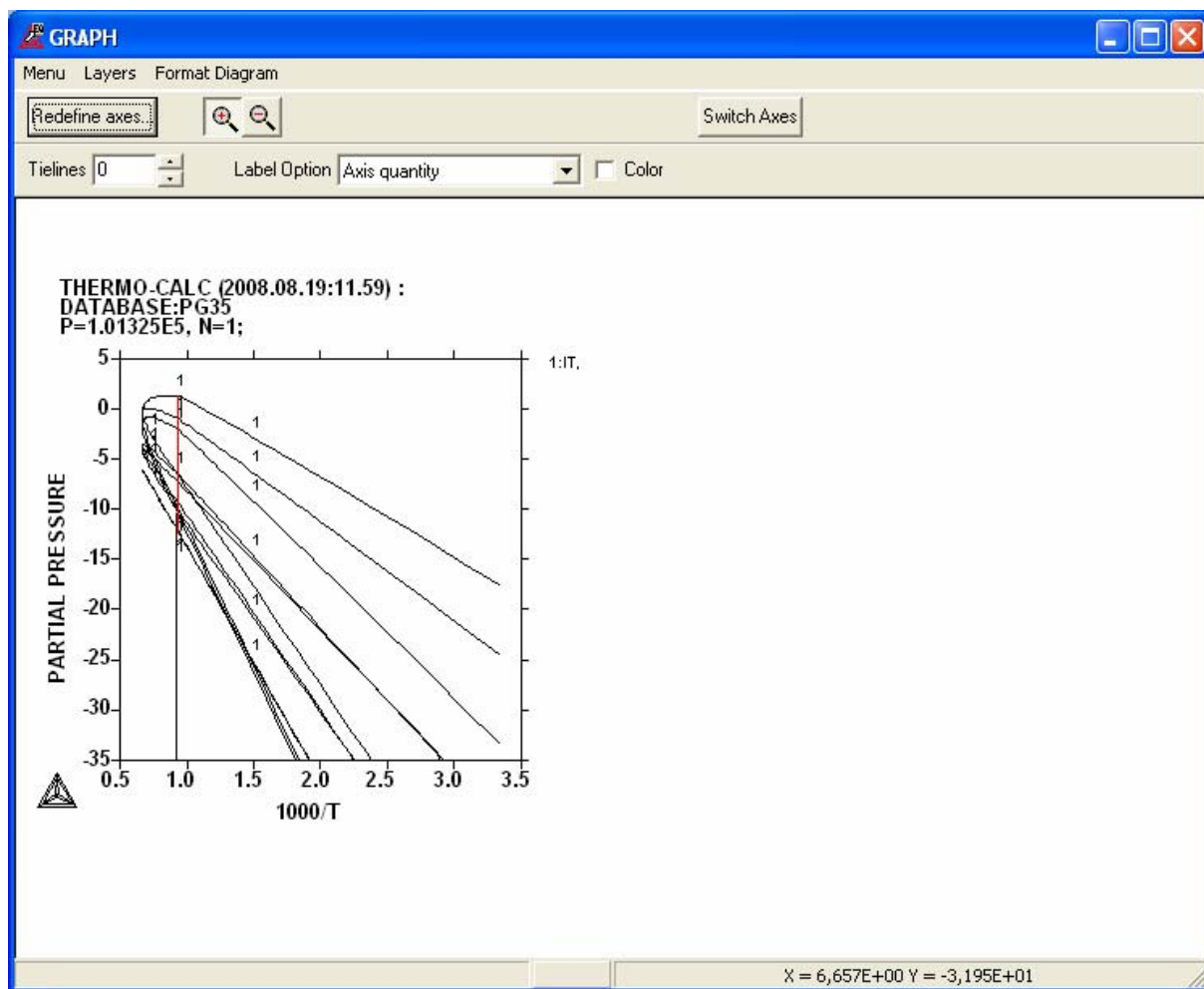
Energy Variables: Additional Quantities:

Partial Derivatives:

User Symbols: **PP**

X-Axis Text: ☒ Automatic Y-Axis Text: ☐ Automatic

Back... ☐ New Graph Window **Next** **Cancel** **Help**

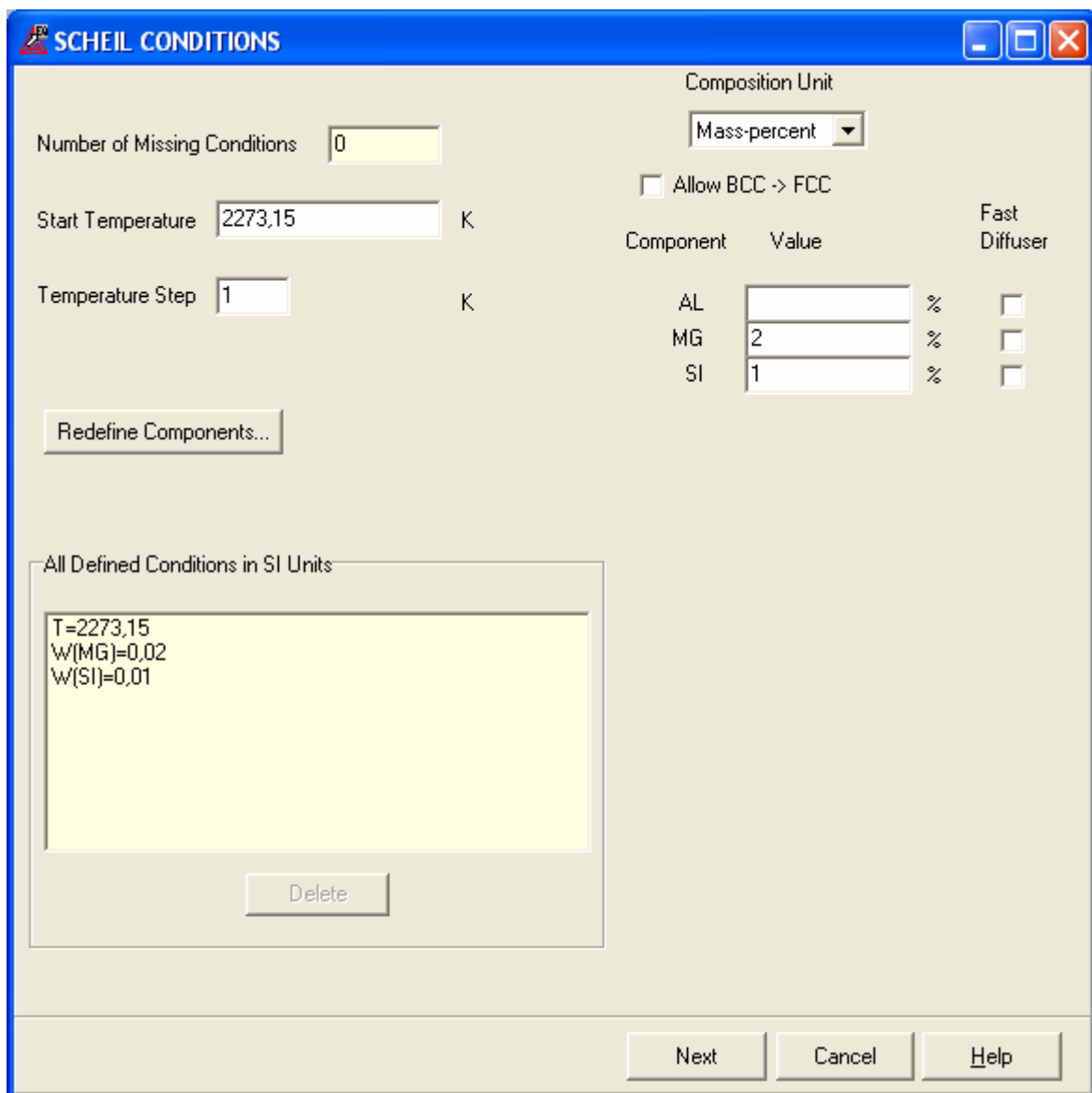


14 Scheil-Gulliver Simulation of Solidification for an Al-Based Alloy

Click  in the MAIN window.

Select *PTERN* from the *Database* list and then click alloy elements *Al*, *Mg*, and *Si* in the periodic table. Click *Next*.

Specify the concentrations of Mg and Si as 2 and 1 *mass-percent*, respectively. Click *Next*.



The dialog box titled "SCHEIL CONDITIONS" contains the following fields and controls:

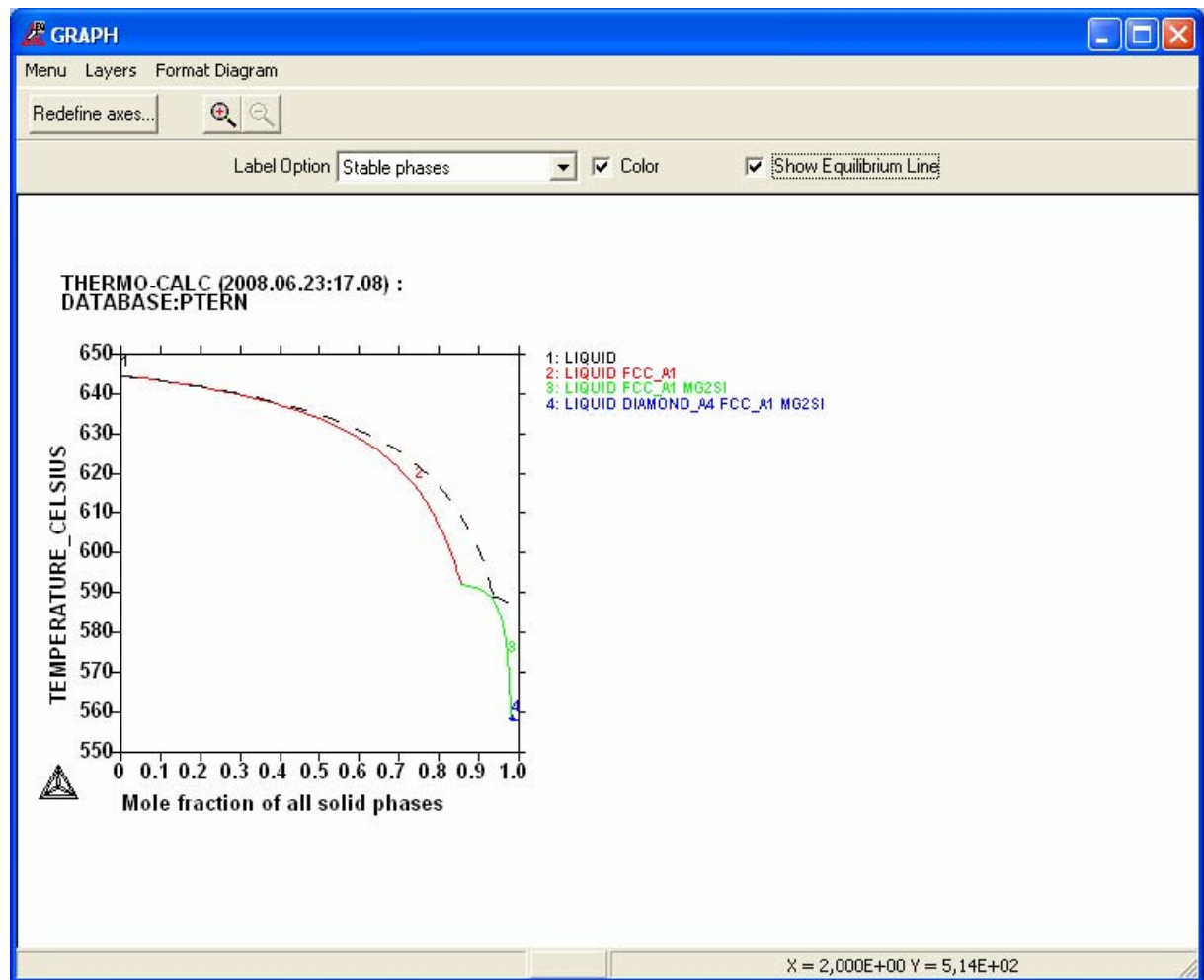
- Number of Missing Conditions:** A text box with the value "0".
- Composition Unit:** A dropdown menu set to "Mass-percent".
- Start Temperature:** A text box with "2273,15" followed by a "K" unit label.
- Temperature Step:** A text box with "1" followed by a "K" unit label.
- Allow BCC -> FCC:** An unchecked checkbox.
- Fast Diffuser:** A column of three checkboxes, all unchecked.
- Component Value Table:**

Component	Value	%
AL		
MG	2	
SI	1	
- Redefine Components...:** A button.
- All Defined Conditions in SI Units:** A text area containing:

```
T=2273,15
W(MG)=0,02
W(SI)=0,01
```
- Delete:** A button below the text area.
- Next, Cancel, Help:** Buttons at the bottom right.

1. Accept the default X and Y –Axis variables by clicking *Next*. The solidification range diagram is plotted.

2. Check the *Show Equilibrium Line* box to add the equilibrium solidification curve.



3. Click *Redefine* and the SCHEIL DIAGRAM window reappears. In the *X-axis* panel, change the *Phase* option to *FCC_A1*. In the *Y-axis* panel, choose *Mass fraction, MG*, and *FCC_A1* under the *Variable*, *For Component*, and *Phase* options, respectively. Enter *Microsegregation of Mg* for the *Diagram Title*. Click *Next*

SCHEIL DIAGRAM

Diagram Axis | Scaling

Diagram Title
Microsegregation of Mg

X-Axis

Variable
NS

For Component Phase
NONE FCC_A1

Axis Text ☒ Automatic
Mole fraction of a solid phase

Y-Axis

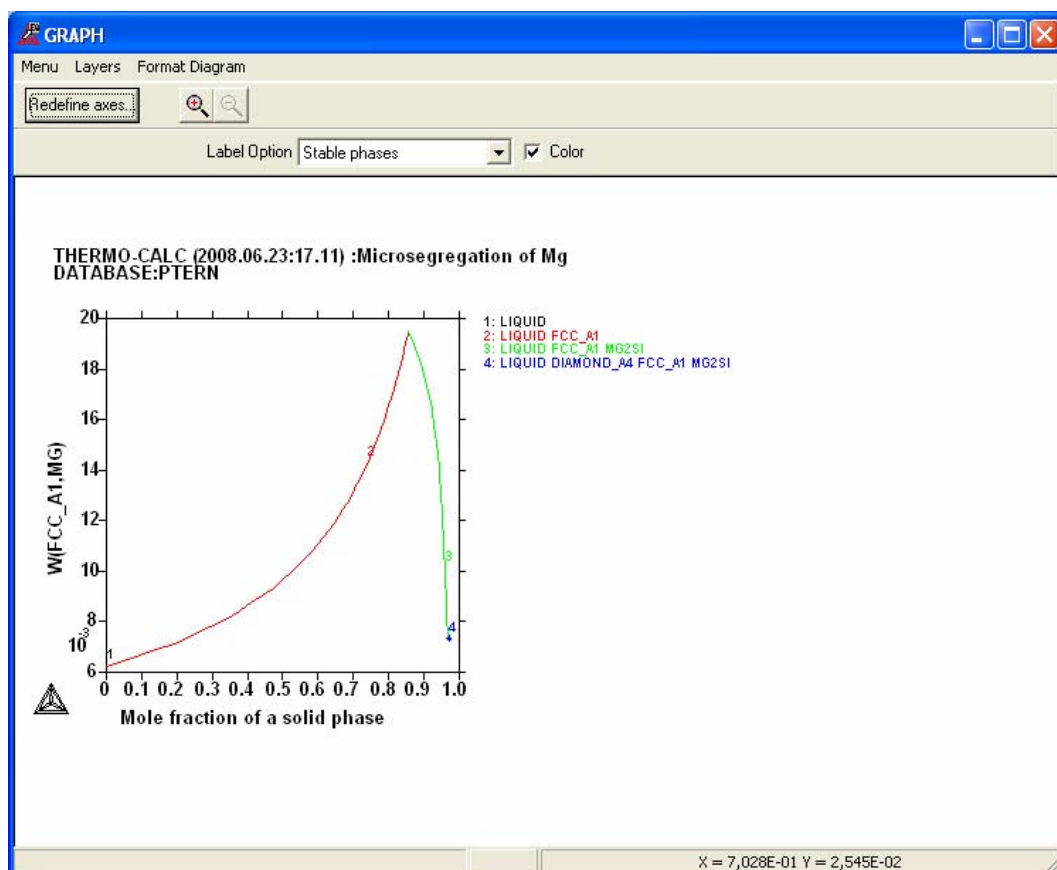
Variable
Mass fraction

For Component Phase
MG FCC_A1


Axis Text ☒ Automatic
W[FCC_A1,MG]

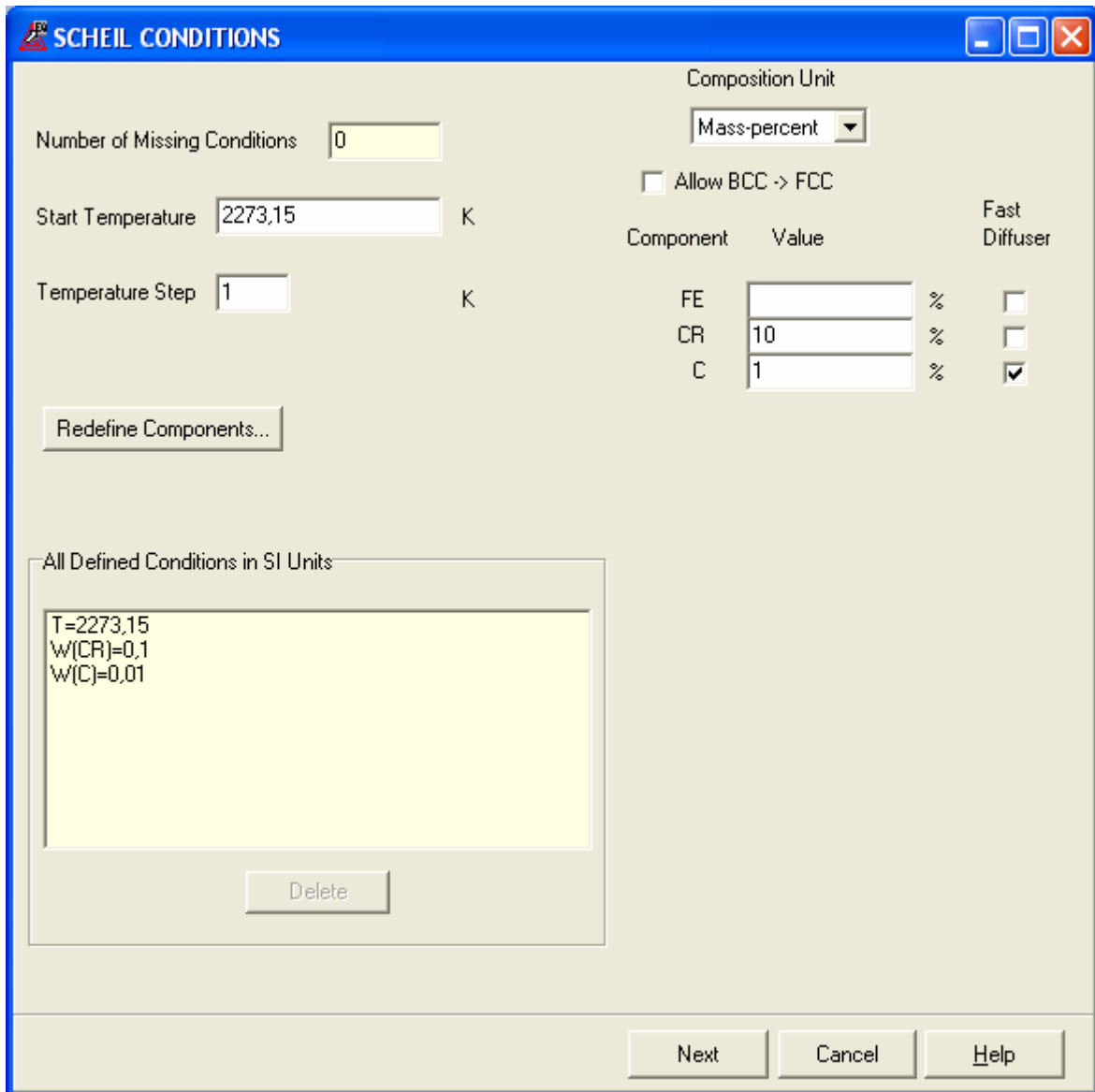
Back... ☐ New Graph Window Next Cancel Help

4. The diagram for the microsegregation of Mg in this alloy is plotted.



15 Scheil-Gulliver Simulation of Solidification for a Steel with Back Diffusion of Carbon in Solid Phases

1. Click  in the MAIN window.
2. Select *PTERN* from the *Database* list and then click alloy elements *Fe*, *Cr*, and *C* in the periodic table. Click *Next*.
3. Specify the concentrations of *C* and *Cr* as *1* and *10 mass-percent*, respectively and check the *Fast Diffuser* box after *C*. Click *Next*.



SCHEIL CONDITIONS

Number of Missing Conditions: 0

Start Temperature: 2273,15 K

Temperature Step: 1 K

Composition Unit: Mass-percent

☐ Allow BCC -> FCC

Component	Value	%	Fast Diffuser
FE		%	<input type="checkbox"/>
CR	10	%	<input type="checkbox"/>
C	1	%	<input checked="" type="checkbox"/>

Redefine Components...

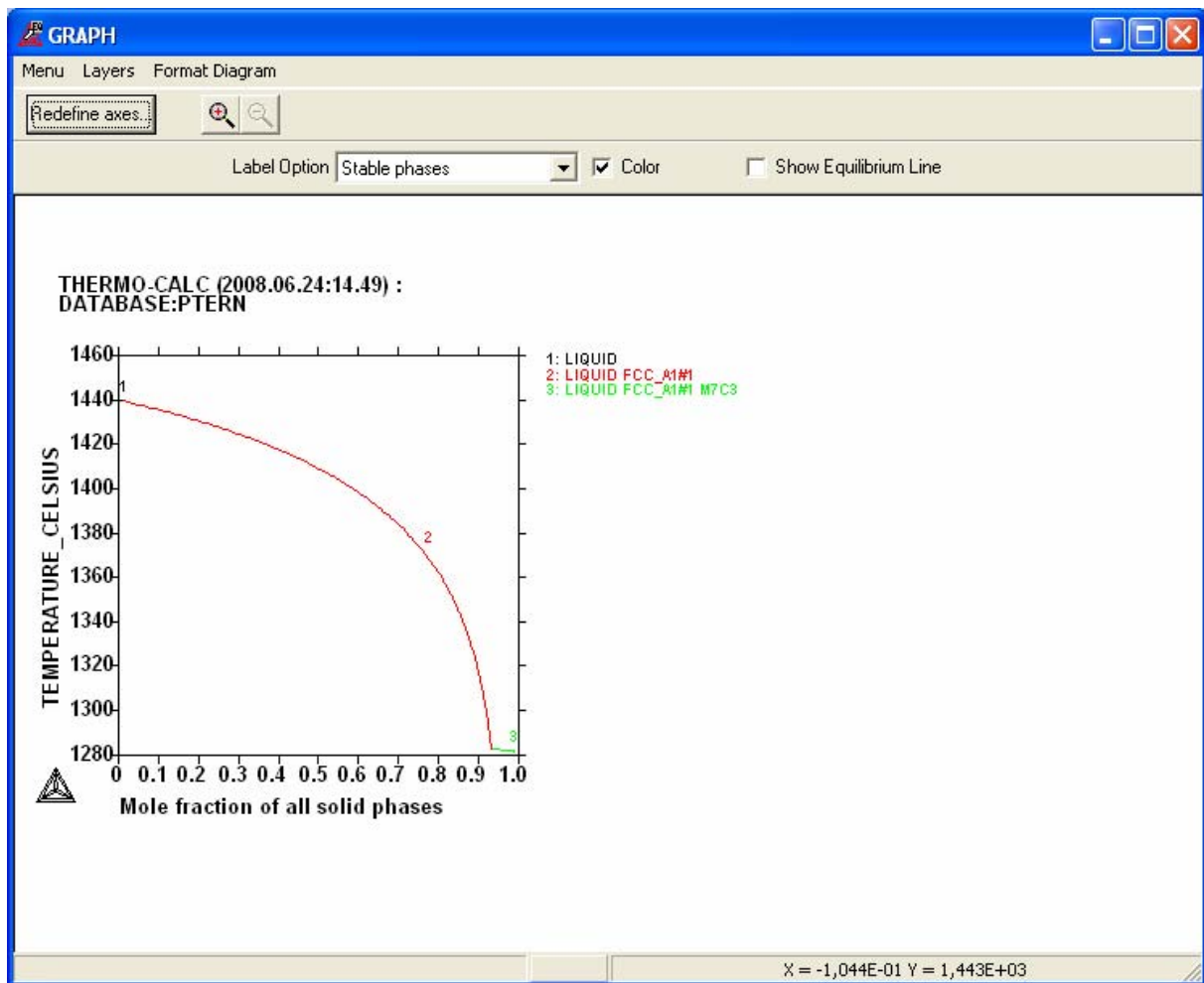
All Defined Conditions in SI Units

T=2273,15
W(CR)=0,1
W(C)=0,01

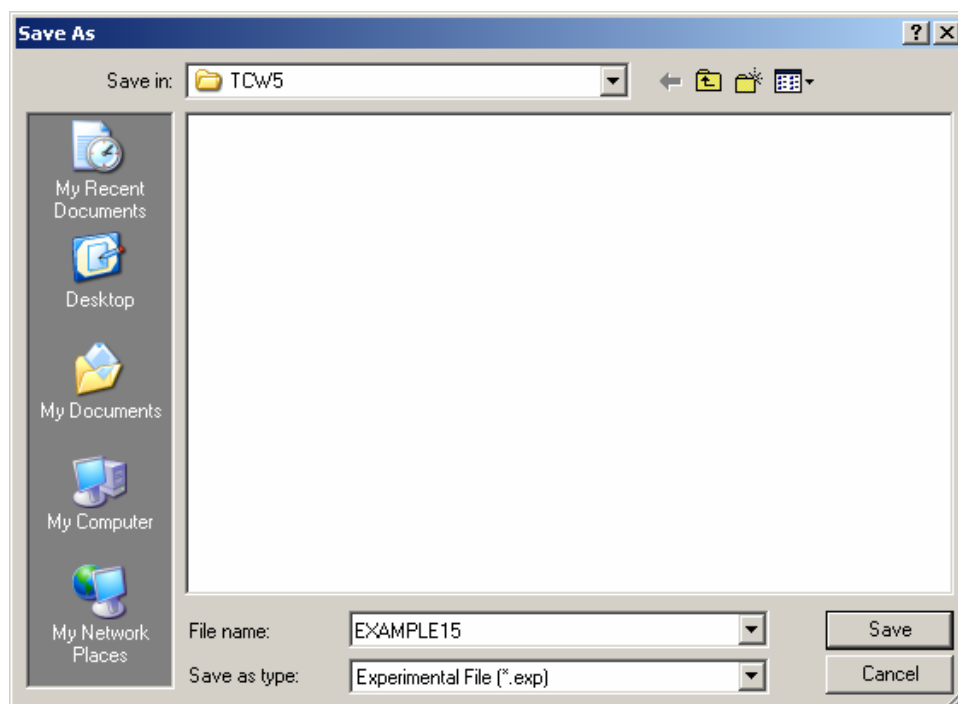
Delete

Next Cancel Help

4. Accept the default X and Y -Axis variables by clicking *Next*. The solidification range diagram is plotted.



5. Click *Menu* → *Save*. Specify file type as Experimental File (*.exp) and file name as EXAMPLE15. Click *Save*.



6. Click *Redefine*. In the *X-axis* panel, change the *Variable* option to *NS* and *Phase* option to *FCC_A1*. In the *Y-axis* panel, choose *Mass fraction*, *CR*, and *FCC_A1* under the *Variable*, *For Component*, and *Phase* options, respectively. Click *Next*.

The screenshot shows the 'SCHEIL DIAGRAM' dialog box with the 'Scaling' tab selected. The 'Diagram Title' field is empty. The 'X-Axis' panel has 'Variable' set to 'NS', 'For Component' set to 'NONE', and 'Phase' set to 'FCC_A1'. The 'Axis Text' field contains 'Mole fraction of a solid phase' and the 'Automatic' checkbox is checked. The 'Y-Axis' panel has 'Variable' set to 'Mass fraction', 'For Component' set to 'CR', and 'Phase' set to 'FCC_A1'. The 'Axis Text' field contains 'W(FCC_A1,CR)' and the 'Automatic' checkbox is unchecked. At the bottom, there are buttons for 'Back...', 'Next', 'Cancel', and 'Help', along with a 'New Graph Window' checkbox.

Diagram Axis | Scaling

Diagram Title

X-Axis

Variable

NS

For Component Phase

NONE FCC_A1

Axis Text ☒ Automatic

Mole fraction of a solid phase

Y-Axis

Variable

Mass fraction

For Component Phase

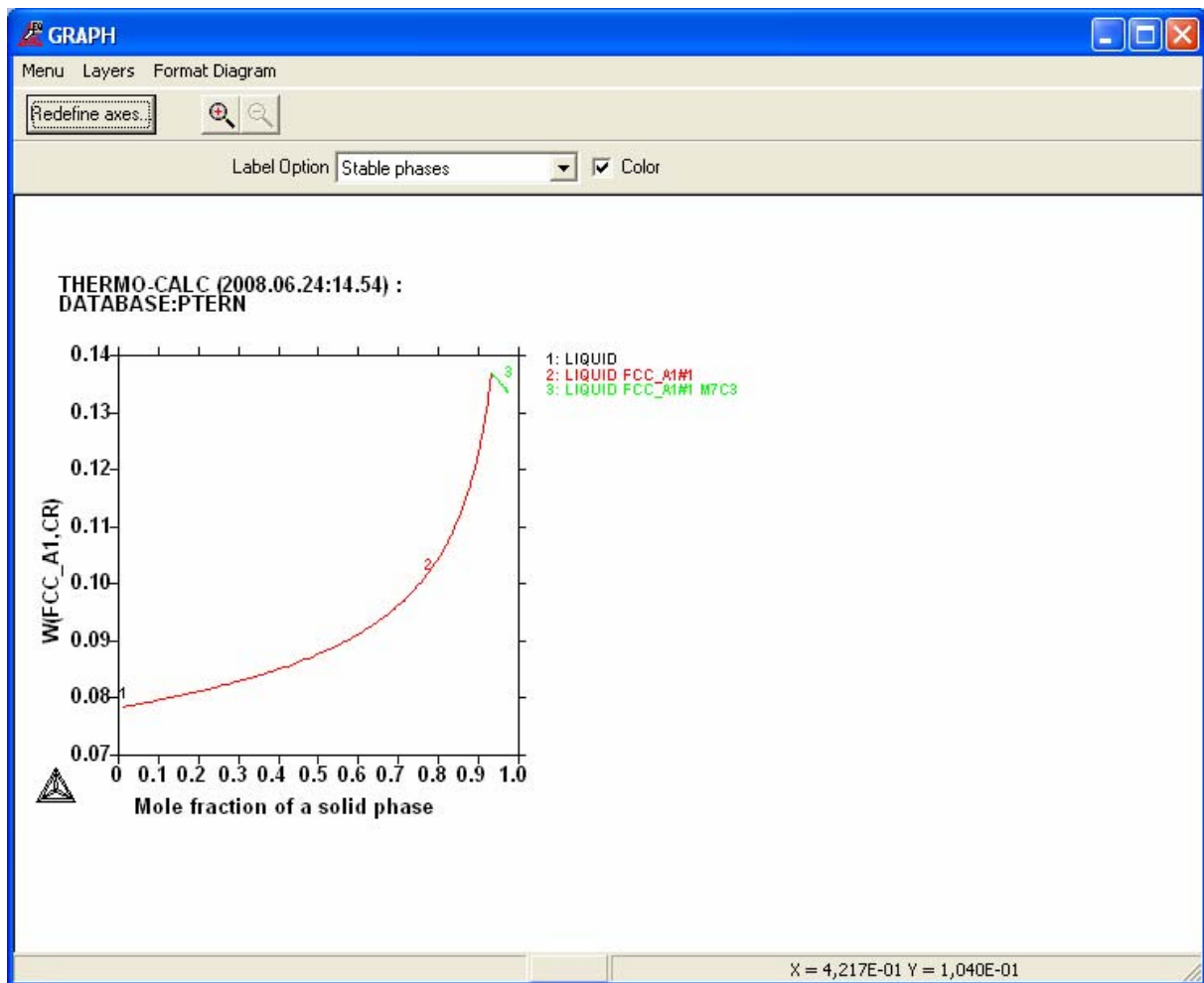
CR FCC_A1


Axis Text ☐ Automatic

W(FCC_A1,CR)

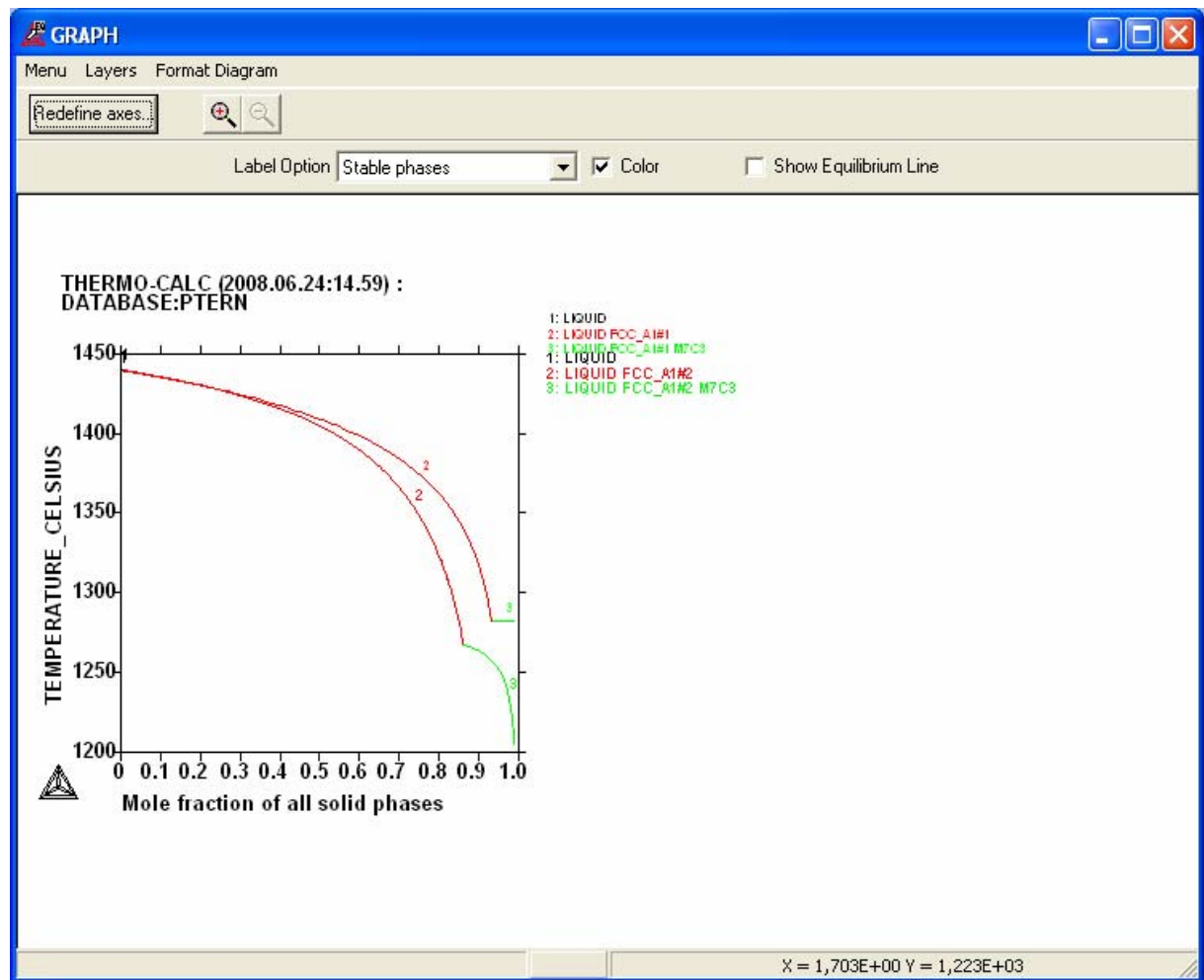
Back... ☐ New Graph Window Next Cancel Help

7. The diagram for the microsegregation of Cr in this alloy is plotted.

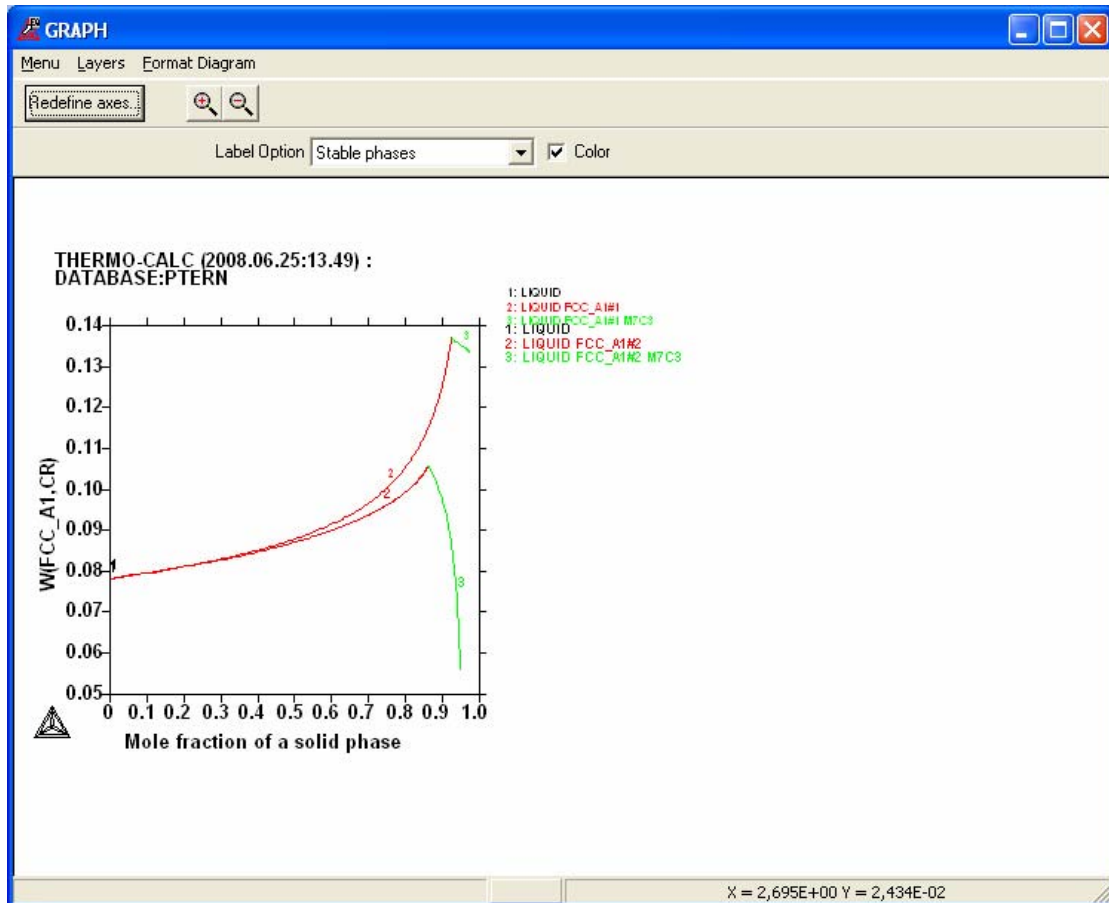
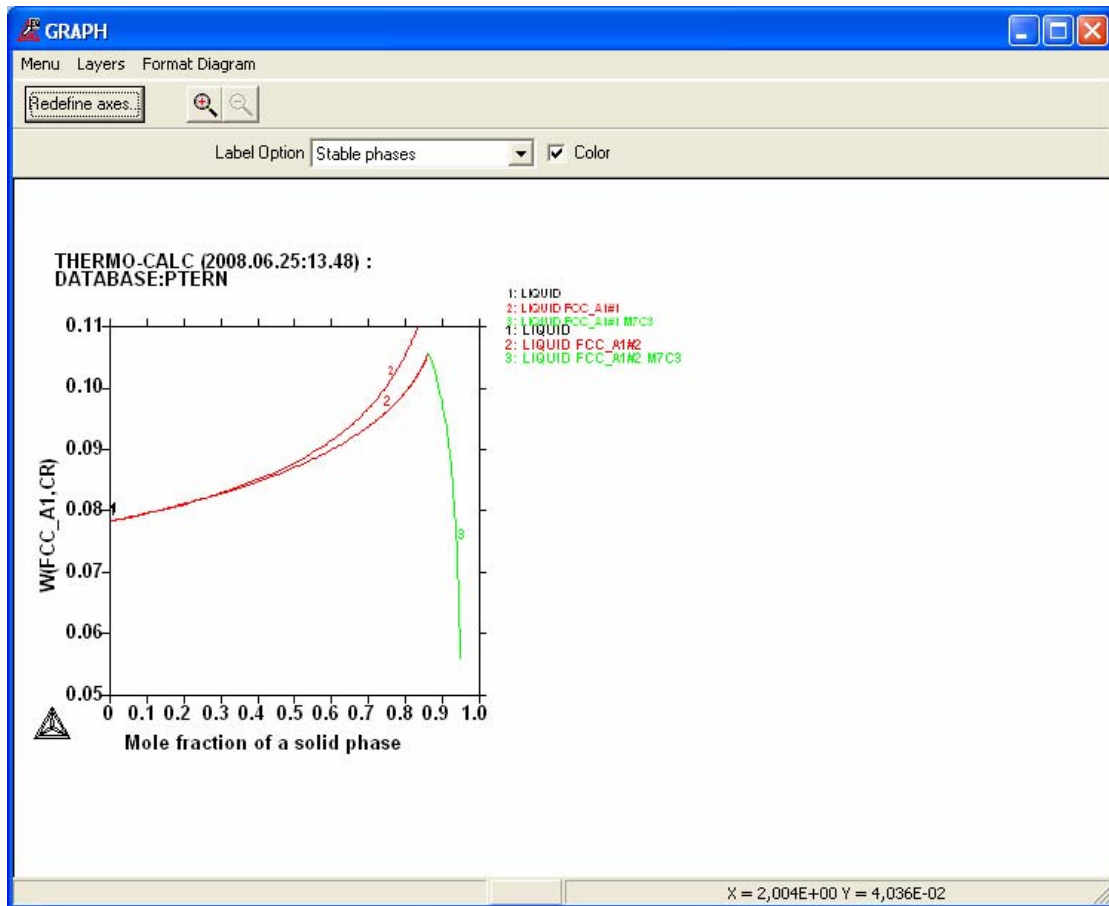


8. Click *Menu* → *Save*. Specify file type as Experimental File (*.exp) and file name as EXAMPLE15_2. Click *Save*.
9. Activate the MAIN window. Click . We are going to do a simple Scheil simulation without considering C back diffusion and compare the results.
10. Click *Next*. The previously selected database and elements has been kept and no need to change.
11. Click *Next*. Enter the same conditions as before (10 mass-percent Cr, 1 mass-percent C and T=2273.15) but keep the interstitial box for C unchecked.
12. Click *Next* to accept default X and Y-axis variables to plot the solidification curve.
13. Click *Menu* → *Append* and then *Add*. Select file *EXAMPLE15.exp* and click *Open* followed by *OK* (make sure the file has the box checked).

14. The solidification curve from the modified Scheil simulation is now superimposed on the result of the simple Scheil simulation.

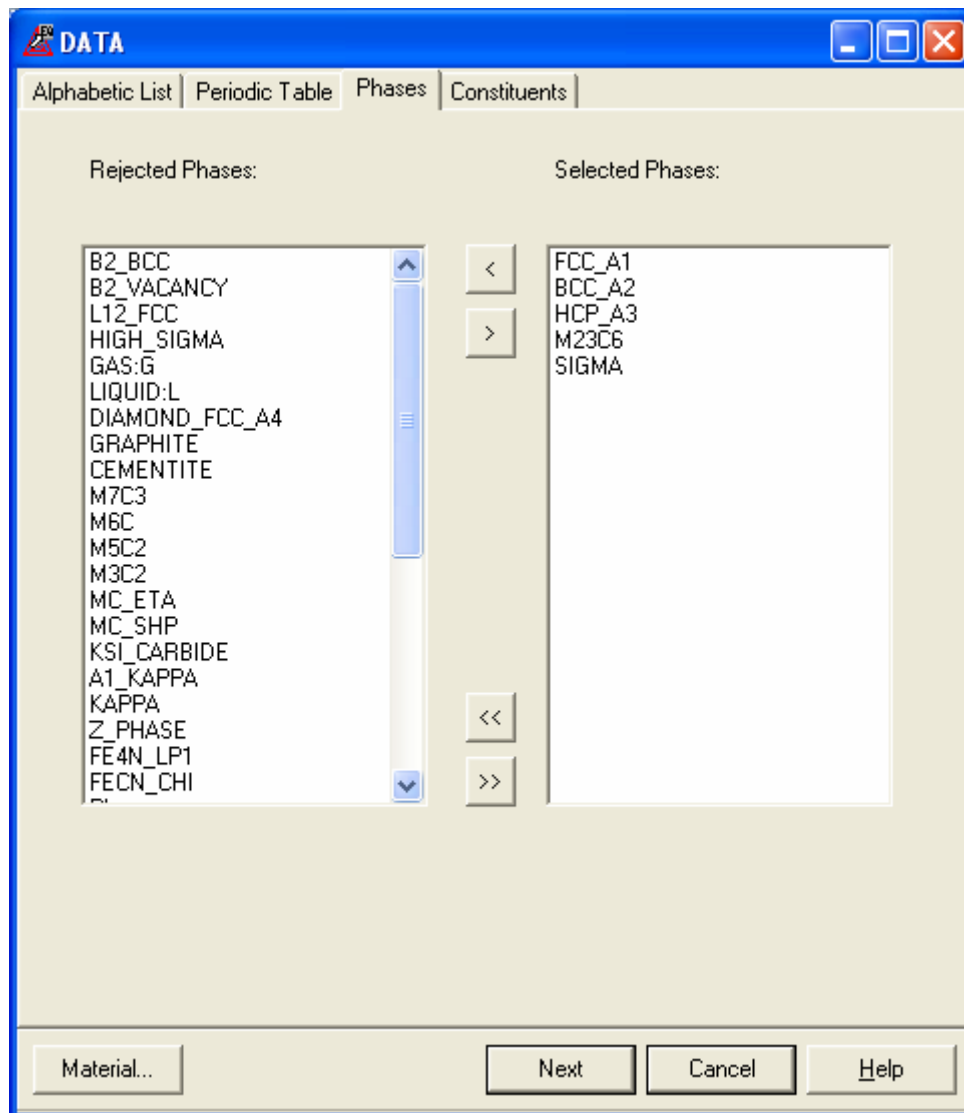


15. Do the same as Steps 9, 10, 11 and 6. Append file *EXAMPLE15_2.exp* in a way similar as in Step 13. One gets a comparison of solute segregation result from the two simulation models.
16. Choose *Scaling...* from the *Format Diagram* menu. Specify the minimum as *0.05* and maximum as *0.11* for the *Y-axis*. Click *Next*. A better scaled diagram is drawn.



16 Calculation of Pitting Resistance Equivalence (PRE) for a Duplex Stainless Steel

1. Click *Elements* in the MAIN window.
2. Select *TCFE6* under the Database option and then click alloy elements *Fe*, *Cr*, *Ni*, *Mo*, *C*, *N*, *Si*, and *Mn* in the periodic table. Select the *Phases* tab. Click to reject all phases first, and then mark the phases *FCC_A1*, *BCC_A2*, *HCP_A3*, *M23C6*, and *SIGMA* and click to restore only these phases.



3. Click *Next*. Specify the concentrations of CR, NI, MO, C, N, SI, and MN as 25, 7, 4, 0.002, 0.27, 0.3, and 0.3, mass-percent respectively. Set start temperature to 1323 K. The default temperature unit can be changed by selecting *Output* in the *Options* menu in the MAIN window.

CONDITIONS

Number of Missing Conditions: 0

Temperature: 1323 K

Pressure: 101325 Pa

System Size: Moles, 1 moles

All Defined Conditions in SI Units:

```

T=1000
P=1.01325E5
N=1
W(CR)=0.25
W(NI)=7E-2
W(MO)=4E-2
W(C)=2E-5
W(N)=2.7E-3
W(SI)=3E-3
W(MN)=3E-3

```

Fixed Phases:

Set Reference State: Components | User Symbols | Start Values

Composition Unit: Mass-percent

Component	Value	Condition
FE		Composition
CR	25	Composition
NI	7	Composition
MO	4	Composition
C	0.002	Composition
N	0.27	Composition
SI	0.3	Composition
MN	0.3	Composition

Buttons: Back... Script Management... Show Value... Compute Next Cancel Help

- Click *Compute*. The phase equilibrium is calculated and the result is shown in a text window.

MAIN

File Edit Applications Script Options Window Help

Elements... Material...

Eq 1

```

BCC_A2#1      STATUS ENTERED      Driving force 0,0000E+00
Number of moles 4,4223E-01, Mass 2,4671E+01
Mass fractions:
FE 6,24173E-01 MO 5,01575E-02 N 3,38915E-04
CR 2,68972E-01 SI 3,51472E-03 C 5,25959E-06
NI 5,03822E-02 MN 2,45631E-03
Constitution:
Sublattice 1 Number of sites 1
FE 6,2437E-01 CR 2,8898E-01 NI 4,7957E-02 MO 2,9206E-02 SI 6,9909E-03 MN 2,4977E-03
Sublattice 2 Number of sites 3
VA 9,9954E-01 N 4,5057E-04 C 8,1543E-06

FCC_A1#1      STATUS ENTERED      Driving force 0,0000E+00
Number of moles 5,5777E-01, Mass 3,0647E+01
Mass fractions:
FE 6,37001E-01 MO 3,18233E-02 SI 2,58565E-03
CR 2,34728E-01 N 4,60067E-03 C 3,18660E-05
NI 8,57922E-02 MN 3,43767E-03
Constitution:
Sublattice 1 Number of sites 1
FE 6,3834E-01 CR 2,5264E-01 NI 8,1807E-02 MO 1,8563E-02 SI 5,1522E-03 MN 3,5019E-03
Sublattice 2 Number of sites 1
VA 9,8147E-01 N 1,8382E-02 C 1,4848E-04
Constitution:
Sublattice 1 Number of sites 1
FE 6,3834E-01 CR 2,5264E-01 NI 8,1807E-02 MO 1,8563E-02 SI 5,1522E-03 MN 3,5019E-03
Sublattice 2 Number of sites 1
VA 9,8147E-01 N 1,8382E-02 C 1,4848E-04

```

5. Select the *Phases* tab on the *CONDITIONS* window. Choose *BCC_A2* and change the *Phase Status* option to *FIXED* with an amount of 0.5 moles. In a similar way, change the phase status of *FCC_A1#2* to *SUSPENDED* in order to avoid possible trouble with this suppose-to-be MC carbide phase during calculation. The system is over-conditioned now and the Degree of Freedom becomes -1. Release the Temperature condition by either removing 1323 in the Temperature box or marking the T=1323 condition in the list of defined conditions and then clicking *Delete*.

CONDITIONS

Number of Missing Conditions: 0

Temperature: K

Pressure: 101325 Pa

System Size: Moles 1 moles

All Defined Conditions in SI Units:

```
P=1.01325E5
N=1
W(CR)=0.25
W(NI)=7E-2
W(MO)=4E-2
W(C)=2E-5
W(N)=2.7E-3
W(SI)=3E-3
W(MN)=3E-3
```

Delete

Fixed Phases:

```
BCC_A2 = 0,50
```

Phases	Status	Moles
BCC_A2	FIXED	0.50
FCC_A1	ENTERED	0.56
FCC_A1#2	SUSPENDED	
HCP_A3	ENTERED	0.00
HCP_A3#2	ENTERED	0.00
M23C6	ENTERED	0.00
SIGMA	ENTERED	0.00
SIGMA#2	SUSPENDED	
SIGMA#3	SUSPENDED	

Phase Status:

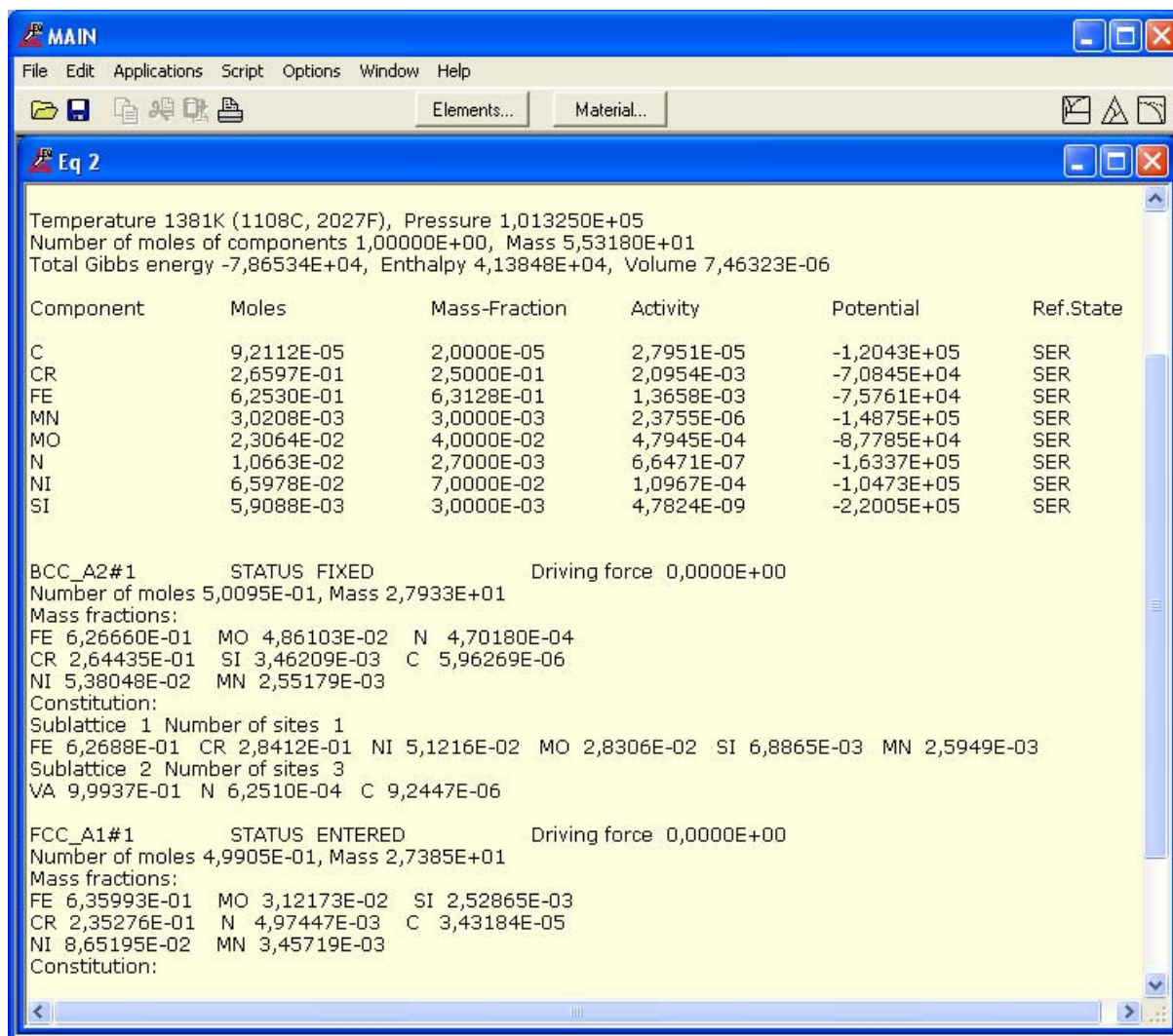
SUSPENDED moles

Phase Conditions...

Add Composition Set...

Back... Script Management... Show Value... Compute Next Cancel Help

6. Click *Compute*. The equilibrium under the defined conditions is calculated. The temperature for developing the duplex structure in this steel is obtained and can be found in the equilibrium result window.



- Go back to the CONDITIONS window and select the *User Symbols* tab to define two PRE functions. In the *Name* box, input *PREFCC*. In the *Expression* box, input $100*W(FCC,CR)+300*W(FCC,MO)+1600*W(FCC,N)$. Click *Add Symbol*. Then, in a similar way, enter the PRE function for BCC_A2, i.e., enter the name *PREBCC* and the expression $100*W(BCC,CR)+300*W(BCC,MO)+1600*W(BCC,N)$.

CONDITIONS

Number of Missing Conditions: 0

Temperature: K

Pressure: 101325 Pa

System Size: Moles 1 moles

All Defined Conditions in SI Units

```
P=1.01325E5
N=1
W(CR)=0.25
W(NI)=7E-2
W(MO)=4E-2
W(C)=2E-5
W(N)=2.7E-3
W(SI)=3E-3
W(MN)=3E-3
```

Delete

Fixed Phases

```
BCC_A2 = 0,50
```

Components

Set Reference State

Advanced Conditions

User Symbols

Phases

Start Values

All Defined Symbols

```
PREFCC=100*W(FCC_A1#1,CR)+300*W(FCC_A1#1,MO)+1
PREBCC=100*W(BCC_A2,CR)+300*W(BCC_A2,MO)+1600*
```

Type: Function

Name:

Expression:

Add Symbol

Delete Symbol

Back... Script Management... Show Value... Compute Next Cancel Help

- Let's have a look of the PRE values now. Click *Show Value*. A window pops up. Choose the function *PREFCC* from the *User Symbols* list and click *Show*. Do same with *PREBCC*. Close the window by clicking *Close*.

SHOW VALUE

Temperature and Pressure:

Potential and Activity:

Compositional Variables:

Phase Variables:

Energy Variables:

Additional Quantities:

Partial Derivatives:

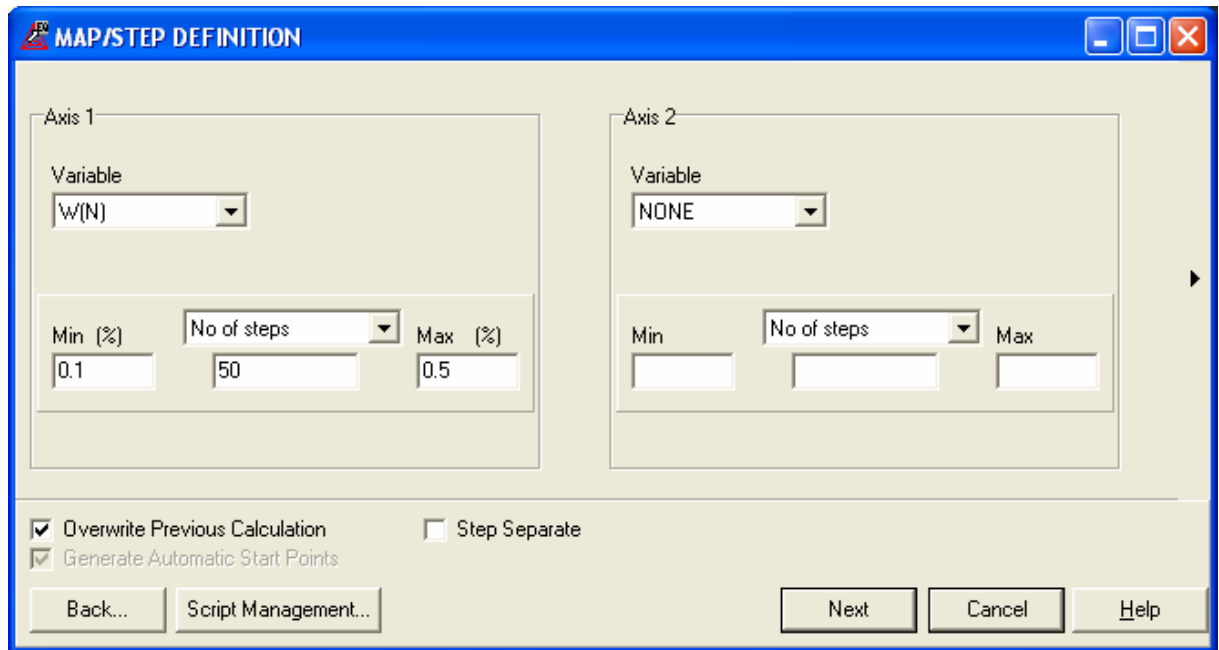
User Symbols:

Show Value of:

Variable	Mnemonic	Value
	PREBCC	41,7789
	PREFCC	40,852

☒ Calculate Equilibrium

- Calculate the PRE of duplex steel with different content of nitrogen. Click *Next* on the CONDITIONS window. The MAP/STEP DEFINITION window appears. Select $W(N)$ for *Axis 1* and change Min value to 0.1 and Max value to 0.5. Click *Next*.



MAP/STEP DEFINITION

Axis 1

Variable:

Min (%): No of steps: Max (%):

Axis 2

Variable:

Min: No of steps: Max:

☒ Overwrite Previous Calculation ☐ Step Separate

☒ Generate Automatic Start Points

Back... Script Management... Next Cancel Help

10. The DIAGRAM DEFINITION window appears. First let's see how the temperature for the formation of duplex structure varies with nitrogen content. Select *Mass Percent* for the X-Axis and *Temperature Kelvin* for the Y-Axis. Click *Next*.

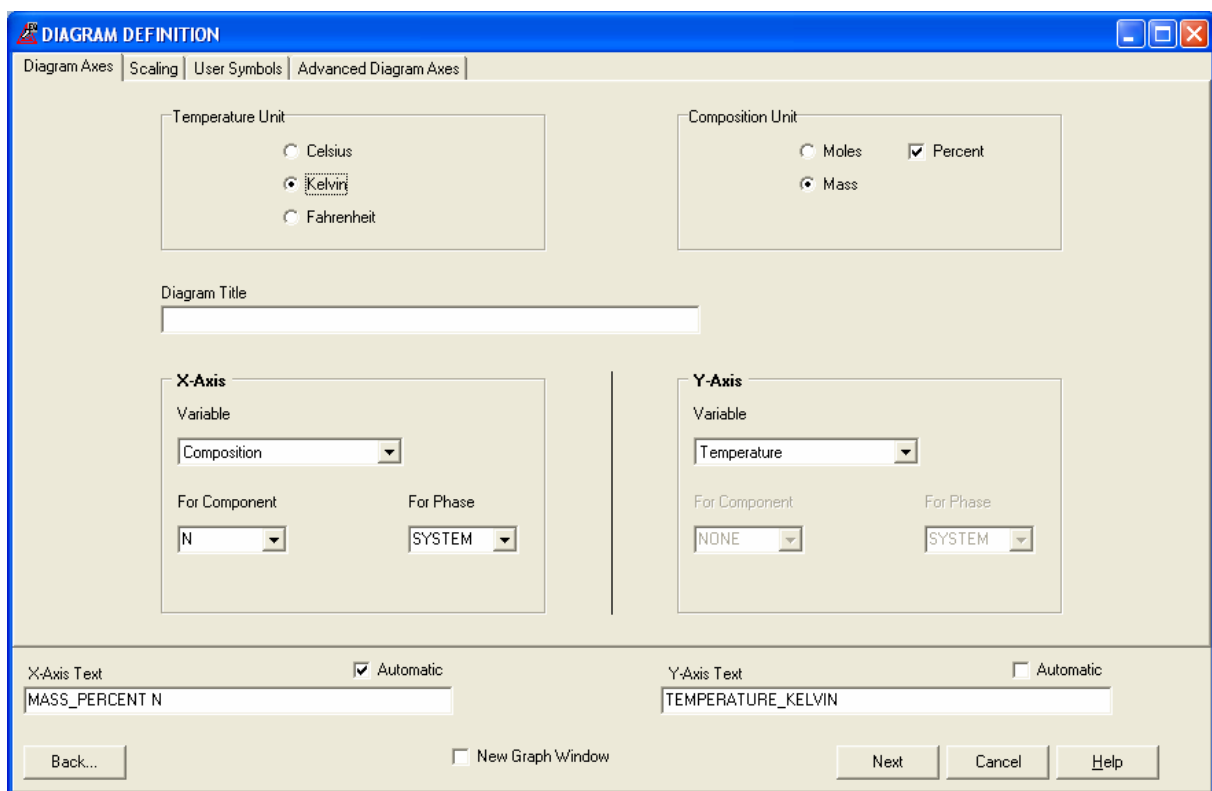


DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | Advanced Diagram Axes

Temperature Unit: ☐ Celsius ☒ Kelvin ☐ Fahrenheit

Composition Unit: ☐ Moles ☒ Percent ☐ Mass

Diagram Title:

X-Axis

Variable:

For Component: For Phase:

Y-Axis

Variable:

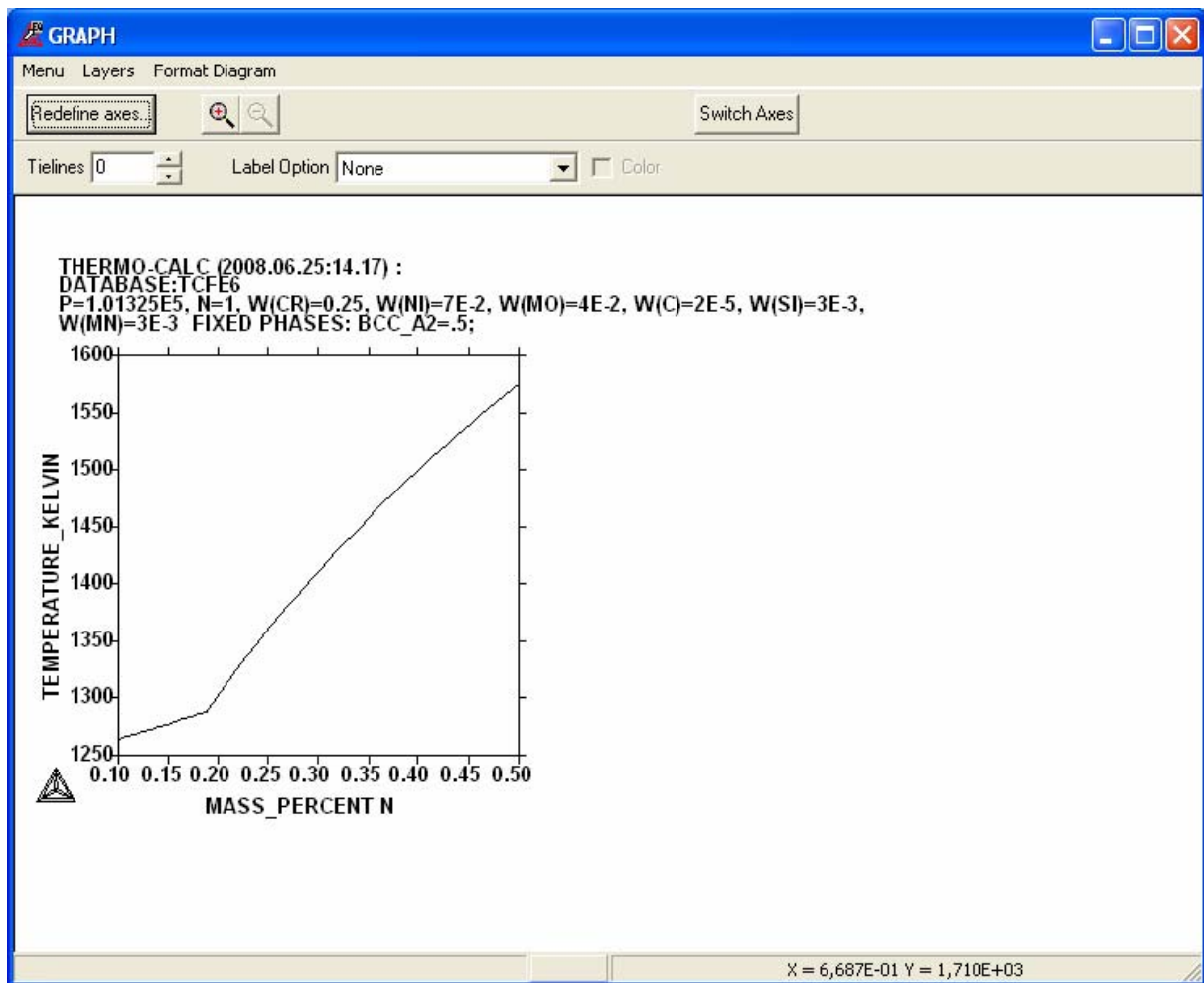
For Component: For Phase:

X-Axis Text: ☒ Automatic

Y-Axis Text: ☐ Automatic

Back... ☐ New Graph Window Next Cancel Help

11. The dependence of temperature on nitrogen concentration is shown for the steel with duplex structure.



12. Click *Redefine*. Select the *User Symbols* tab. Change symbol *Type* to *Table*. Enter name *PREFB*. Enter expression *PREFCC*, *PREBCC*, click *Add Symbol*.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | **Advanced Diagram Axes**

All Defined Symbols

```

PREFCC=100*w/(FCC_A1#1,CR)+300*w/(FCC_A1#1,MO)+1
PREBCC=100*w/(BCC_A2,CR)+300*w/(BCC_A2,MO)+1600*
PREFB=PREFCC,PREBCC

```

Type: **Table** Name:

Expression:

Add Symbol **Delete Symbol** **Tabulate**

X-Axis Text: ☒ Automatic Y-Axis Text: ☐ Automatic

Back... ☐ New Graph Window **Next** **Cancel** **Help**

13. Select *Advanced Diagram Axes* tab. Select *PREFB* as Y-Axis Variable. Click *next* to plot.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | **Advanced Diagram Axes**

Diagram Title:

X-Axis

Temperature and Pressure: Potential and Activity:

Compositional Variables: **Mass-percent** Phase Variables:

Energy Variables: Additional Quantities:

Partial Derivatives:

User Symbols:

Y-Axis

Temperature and Pressure: Potential and Activity:

Compositional Variables: Phase Variables:

Energy Variables: Additional Quantities:

Partial Derivatives:

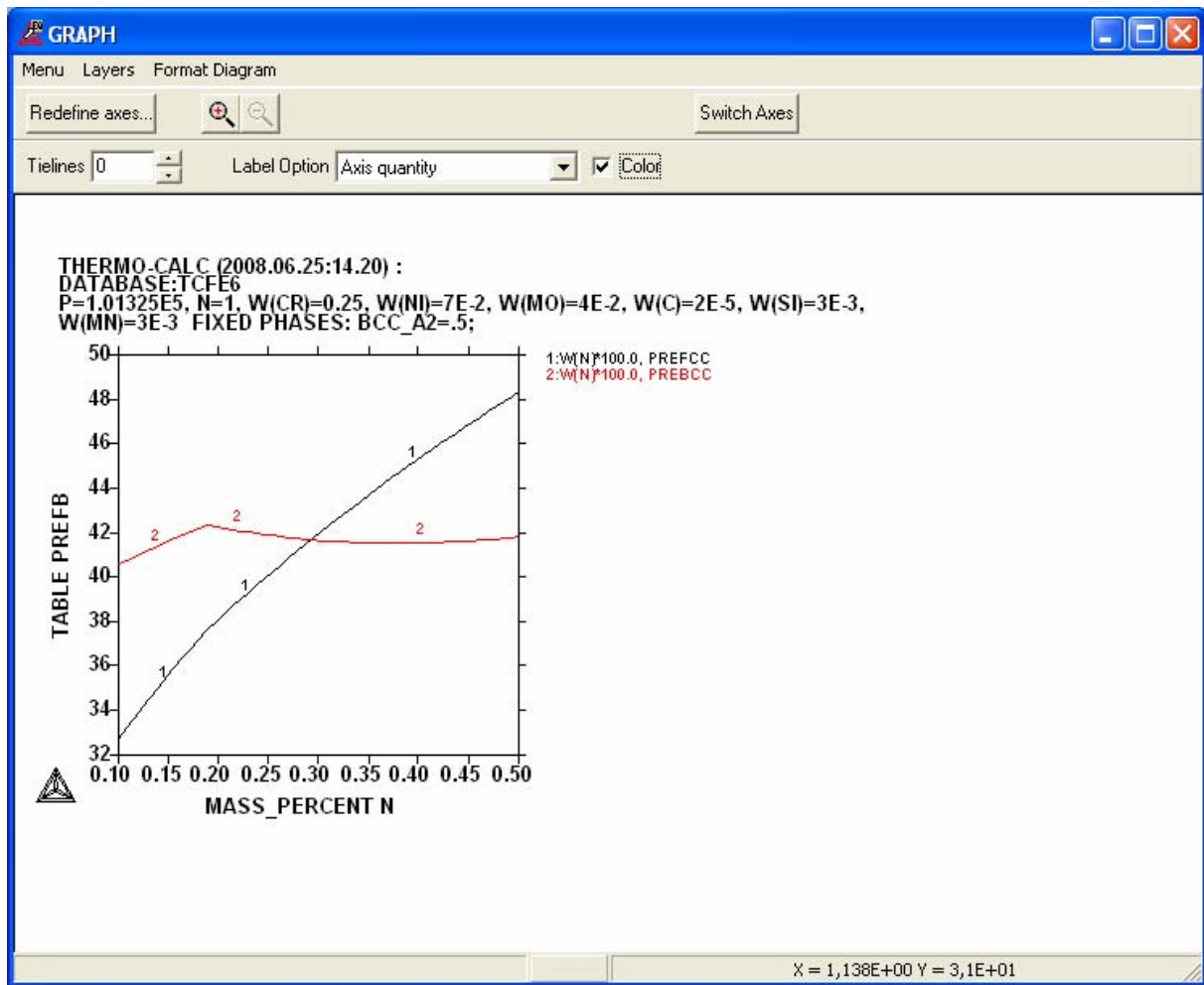
User Symbols: **PREFB**

For Component: **N**

X-Axis Text: ☒ Automatic Y-Axis Text: ☒ Automatic

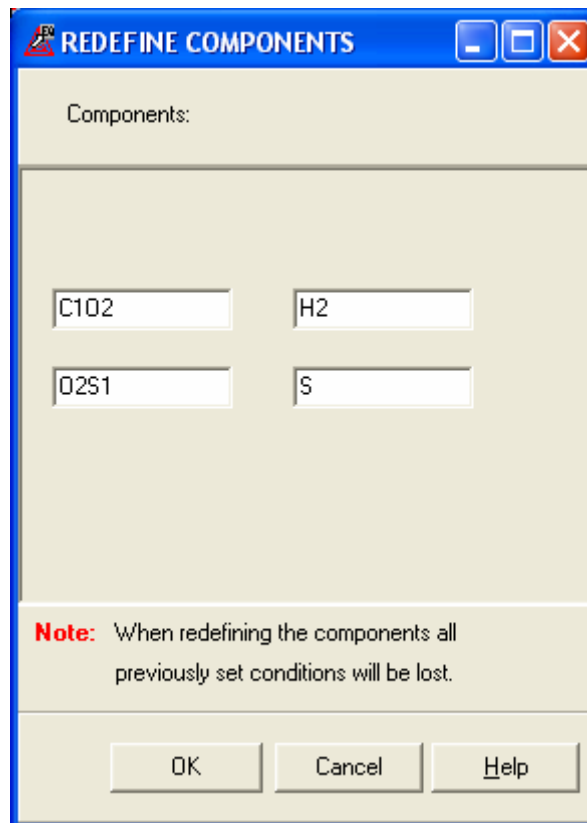
Back... ☐ New Graph Window **Next** **Cancel** **Help**

14. Choose *Axis quantity* in the *Label Option* menu and check the *Color* box.



17 Calculation of Speciation of a Gas

1. Click *Elements* in the MAIN window.
2. Select *SSUB4* from the Database list and then click elements *C*, *H*, *O*, and *S* in the periodic table. Click *Next*.
3. Click *Redefine*. In the REDEFINE COMPONENTS window, change *C* to *C1O2*, *H* to *H2*, *O* to *O2S1*. Click *OK*.



4. Select *Moles* as *Default Unit*. Enter value *5* for *C1O2*, *10* for *H2*, *0.1* for *O2S1*, and *0* for *S*. Set the temperature to *750 °C* and the pressure to *1E5*. Click *Next*.

CONDITIONS

Number of Missing Conditions: 0

Temperature: 750 C

Pressure: 100000 Pa

System Size: Moles

All Defined Conditions in SI Units:

```
N(H2)=10
N(C102)=5
N(O2S1)=0.1
N(S)=0
T=1023.15
P=1E5
```

Delete

Fixed Phases:

Set Reference State | User Symbols | Start Values

Components | Advanced Conditions | Phases

Composition Unit: Moles

Component	Value	Condition
C102	5	Composition
H2	10	Composition
O2S1	0.1	Composition
S	0	Composition

Back... Script Management... Show Value... Compute Next Cancel Help

- Keep the temperature variable for *Axis 2* and change the variable of *Axis 1* to *NONE*.

MAP/STEP DEFINITION

Axis 1

Variable: NONE

Min: No of steps: Max:

Axis 2

Variable: T

Min (C): 500 No of steps: 50 Max (C): 2000

☒ Overwrite Previous Calculation ☐ Step Separate

☒ Generate Automatic Start Points

Back... Script Management... Next Cancel Help

- Click *Next*. A stepping calculation is performed and the **DIAGRAM DEFINITION** window appears. The default axes are *Temperature Celsius* and *Phase Fraction* for all phases. Keep these axes and click *Next*.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | Advanced Diagram Axes

Temperature Unit
☒ Celsius
☐ Kelvin
☐ Fahrenheit

Composition Unit
☒ Moles ☐ Percent
☐ Mass

Diagram Title

X-Axis
 Variable:
 For Component: For Phase:

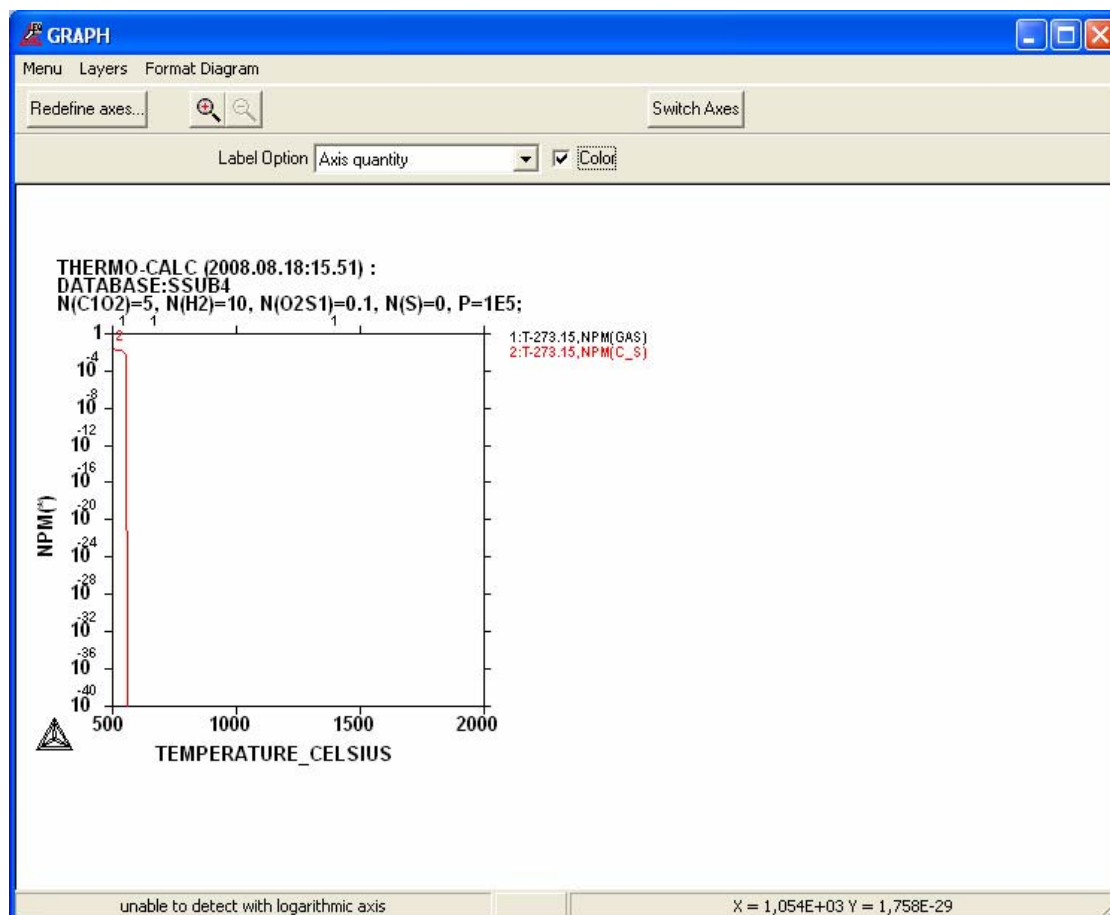
Y-Axis
 Variable:
 For Component: For Phase:

X-Axis Text ☒ Automatic

Y-Axis Text ☒ Automatic

Back... ☐ New Graph Window Next Cancel Help

- Click *Next* to plot the diagram. Choose *Logarithmic Y-axis* in the *Format Diagram* menu. Select *Axis quantity* in the *Label Option* menu and check the *Color* box.



- Click *Redefine*. Go to the *Advanced Diagram Axes* tab and select *Phase Constitution* for all species in the *GAS* phase as the Y-axis.

DIAGRAM DEFINITION

Diagram Axes | Scaling | User Symbols | **Advanced Diagram Axes**

Diagram Title

X-Axis

Temperature and Pressure: **Temperature Celsius**

Potential and Activity: []

Compositional Variables: []

Phase Variables: []

Energy Variables: []

Additional Quantities: []

Partial Derivatives: []

User Symbols: []

Y-Axis

Temperature and Pressure: []

Potential and Activity: []

Compositional Variables: []

Phase Variables: **Phase Constitution**

Energy Variables: []

Additional Quantities: []

Partial Derivatives: []

User Symbols: []

For Species: **ALL**

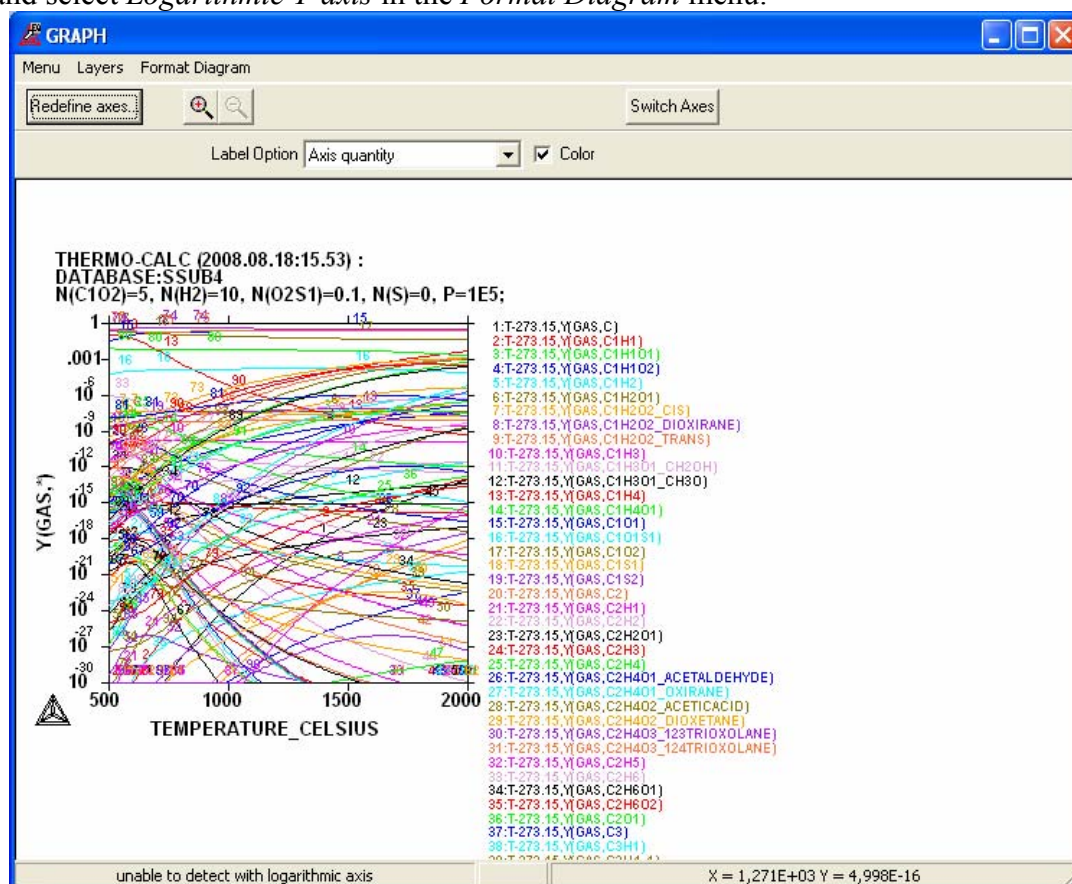
For Phase: **GAS**

X-Axis Text: **TEMPERATURE_CELSIUS** ☒ Automatic

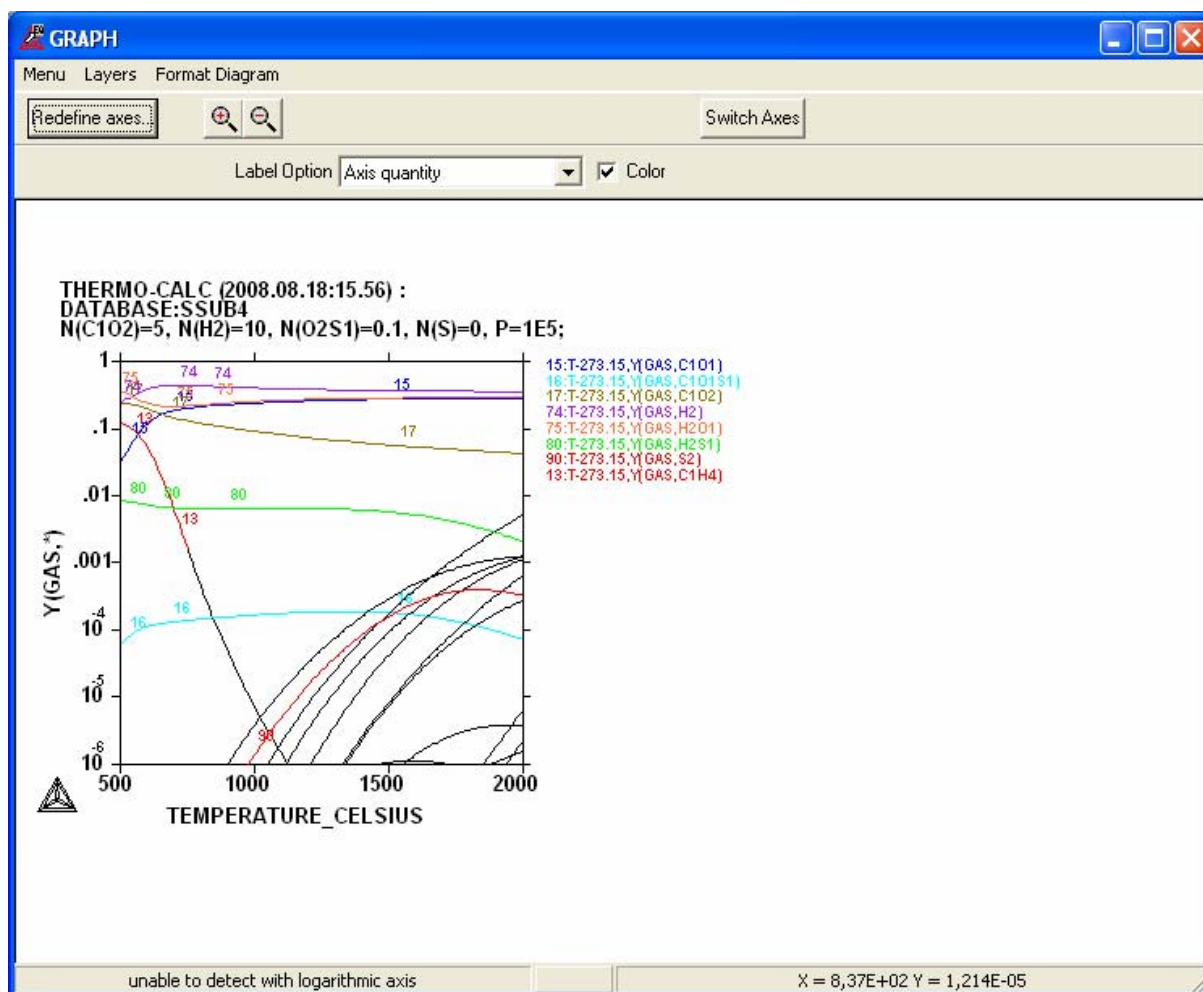
Y-Axis Text: **Y[GAS,']** ☒ Automatic

Back... ☐ New Graph Window Next Cancel Help

- Click *Next* to plot. Select *Axis quantity* in the *Label Option* menu, check the *Color* box and select *Logarithmic Y-axis* in the *Format Diagram* menu.

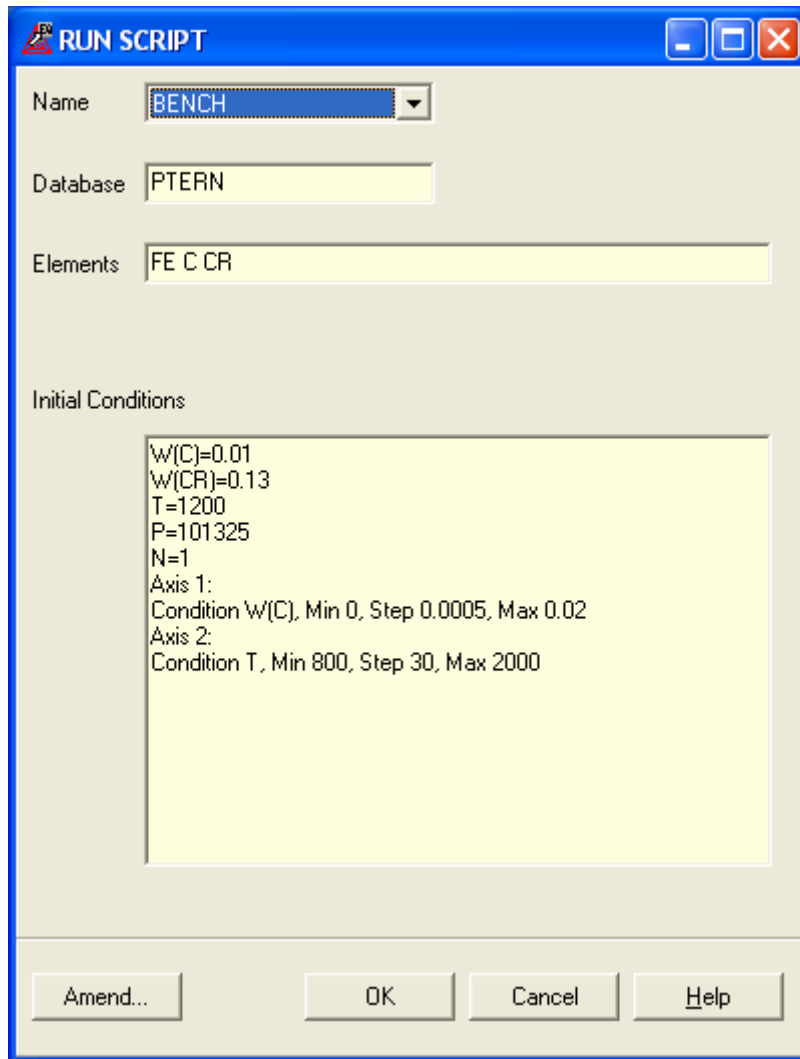


10. Choose *Scaling...* from the *Format Diagram* menu. Change the Min value to $1E-6$ and Max to 1 on the *Y-Axis* panel. Click next to plot.

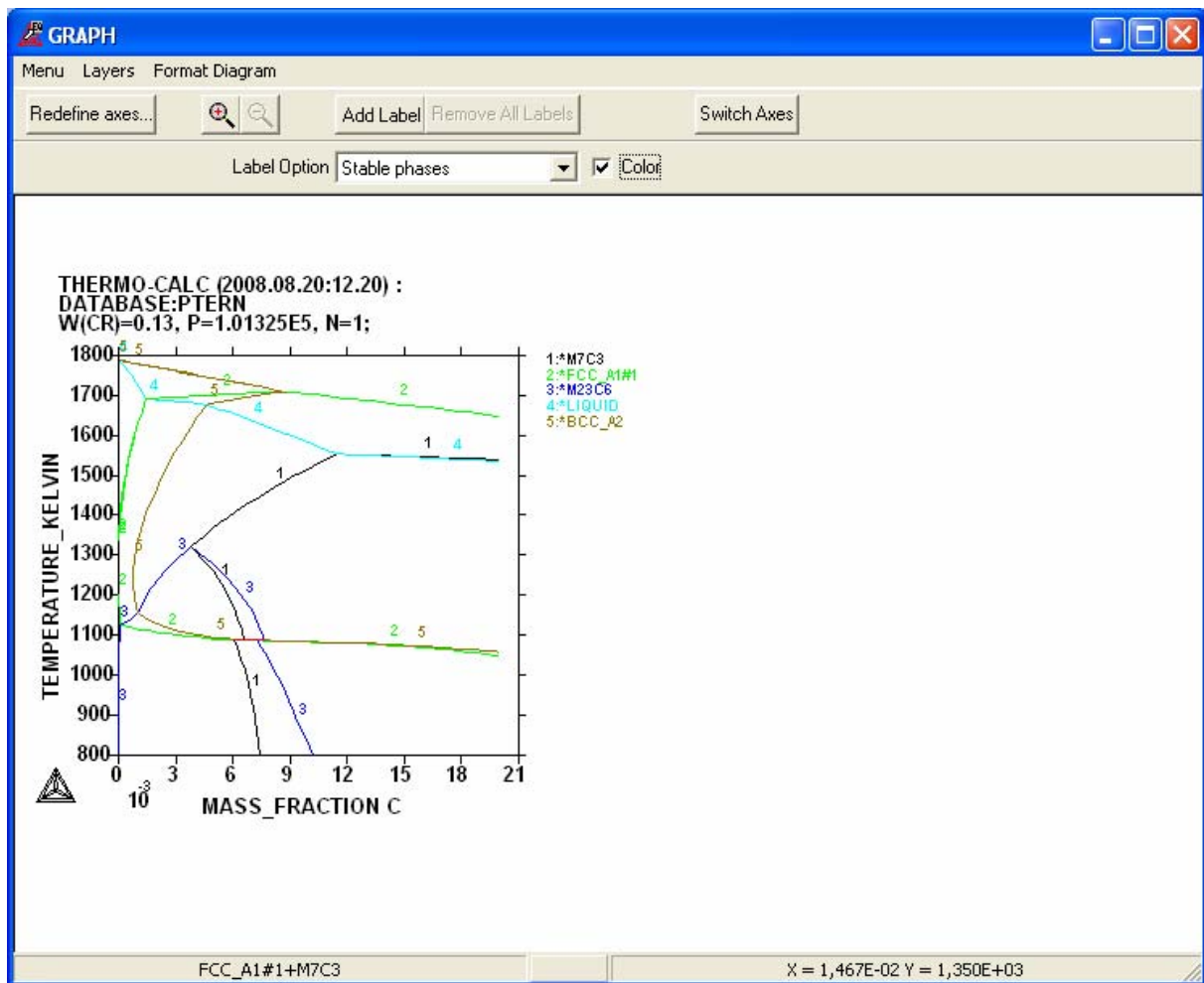


18 Calculation Using Script and how to Implement a Figure to a Word/PowerPoint file

1. Start TCW and select the *Script* tab in the MAIN window.
2. Choose *Run Script* under the *Script* tab and select the *Name* BENCH. Click *OK*.



3. Select *Stable phases* in the *Label Option* menu and check the *Color* box.



4. To create your own Script select *Script Management* under the *Script* tab in the MAIN window. Click on *New Script*.
5. Give the new Script the *Name* EXAMPLE18 and select e.g. the TCFE6 Database. Define Fe, C, Cr, Si, and Mo in the *Components* box and click the *Add* button. Enter T in the *Condition* box and give it the value 1200. Click the *Add* button. Repeat the last procedure to enter the composition of the defined system; W(C)=0.005, W(Cr)=0.02, W(Si)=0.004, W(Mo)=0.014. To fulfill all the degrees of freedom one must define the pressure, P=101325, and the size of the system, N=1.
6. Enter T as *Condition* for *Axis 1* with min 600 and max 2000 with a step length of 20. Click *Save*.

SCRIPT MANAGEMENT

Name:

Database:

Components:

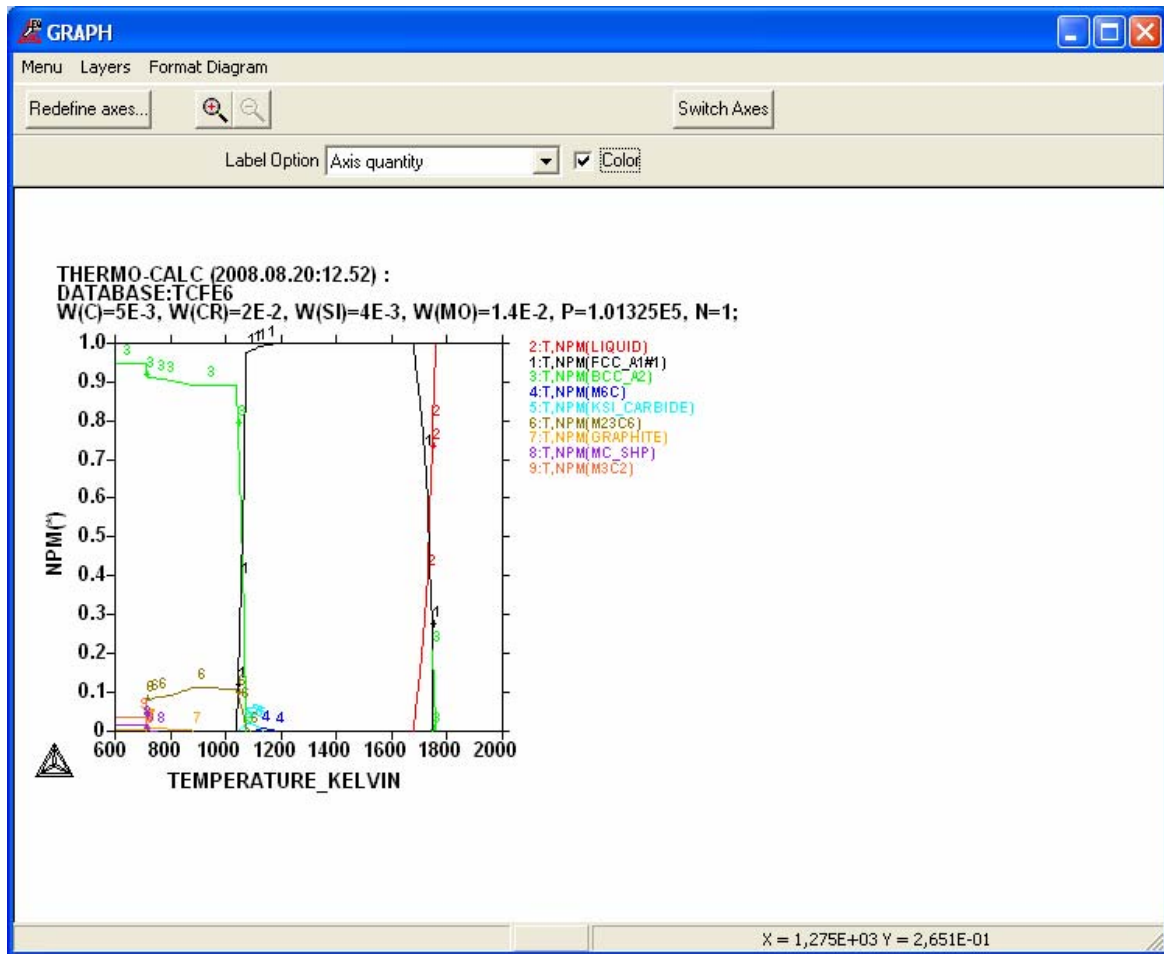
Condition: Value:

Info:

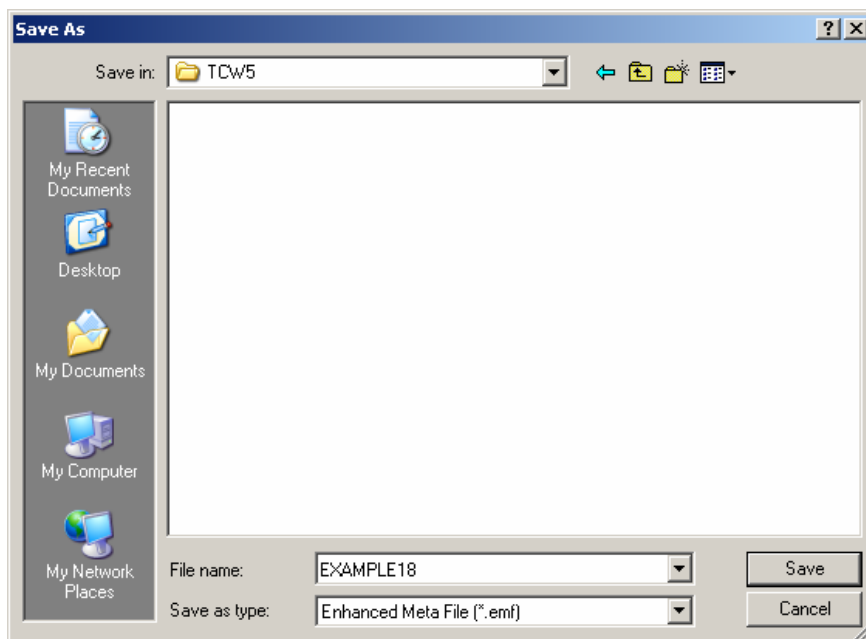
Name: EXAMPLE18
 Database: TCFE6
 Components: FE C CR SI MO
 Conditions:
 T=1200
 W(C)=0.005
 W(CR)=0.02
 W(SI)=0.004
 W(MO)=0.014
 P=101325
 N=1
 Axis1:
 Condition T, Min 600, Step 20, Max 2000

Axis	Condition	Min	Step	Max
Axis1	<input type="text" value="T"/>	<input type="text" value="600"/>	<input type="text" value="20"/>	<input type="text" value="2000"/>
Axis2	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
Axis3	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>

7. Choose *Run Script* under the *Script* tab in the MAIN window and select the *Name* EXAMPLE18. Click *OK* (the *Amend* button take you to the CONDITIONS window). Select *Axis quantity* in the *Label Option* menu and check the *Color* box.



- Click *Menu* → *Save*. Specify file type as e.g. Enhanced Meta File (*.emf) and file name as EXAMPLE18. Click *Save*.



- Implement the figure into a Word/PowerPoint file using *Picture*→*From File* under the *Insert* tab (in Word or PowerPoint).