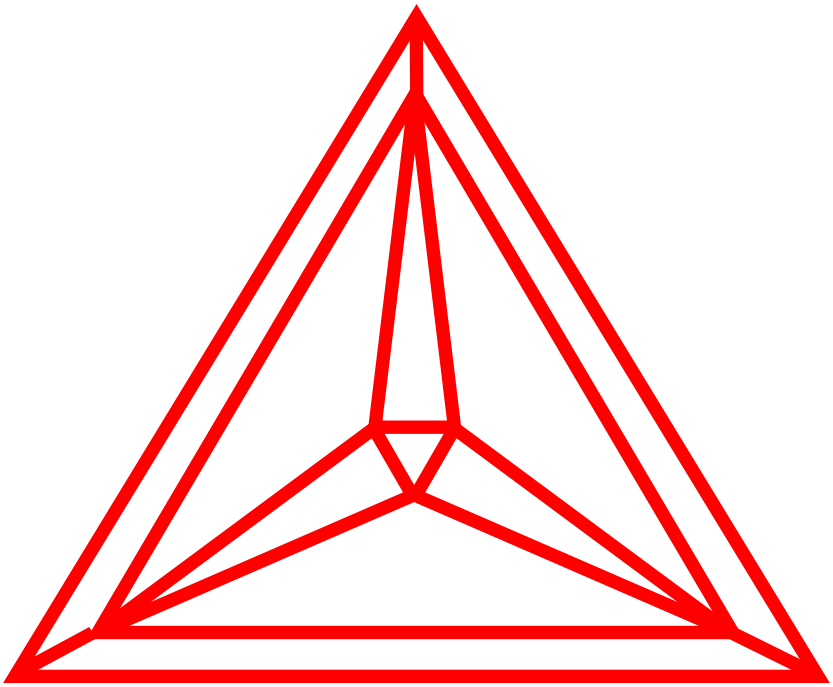
TCW™

(Thermo-Calc® Windows)

Examples Book

Version 5.0



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

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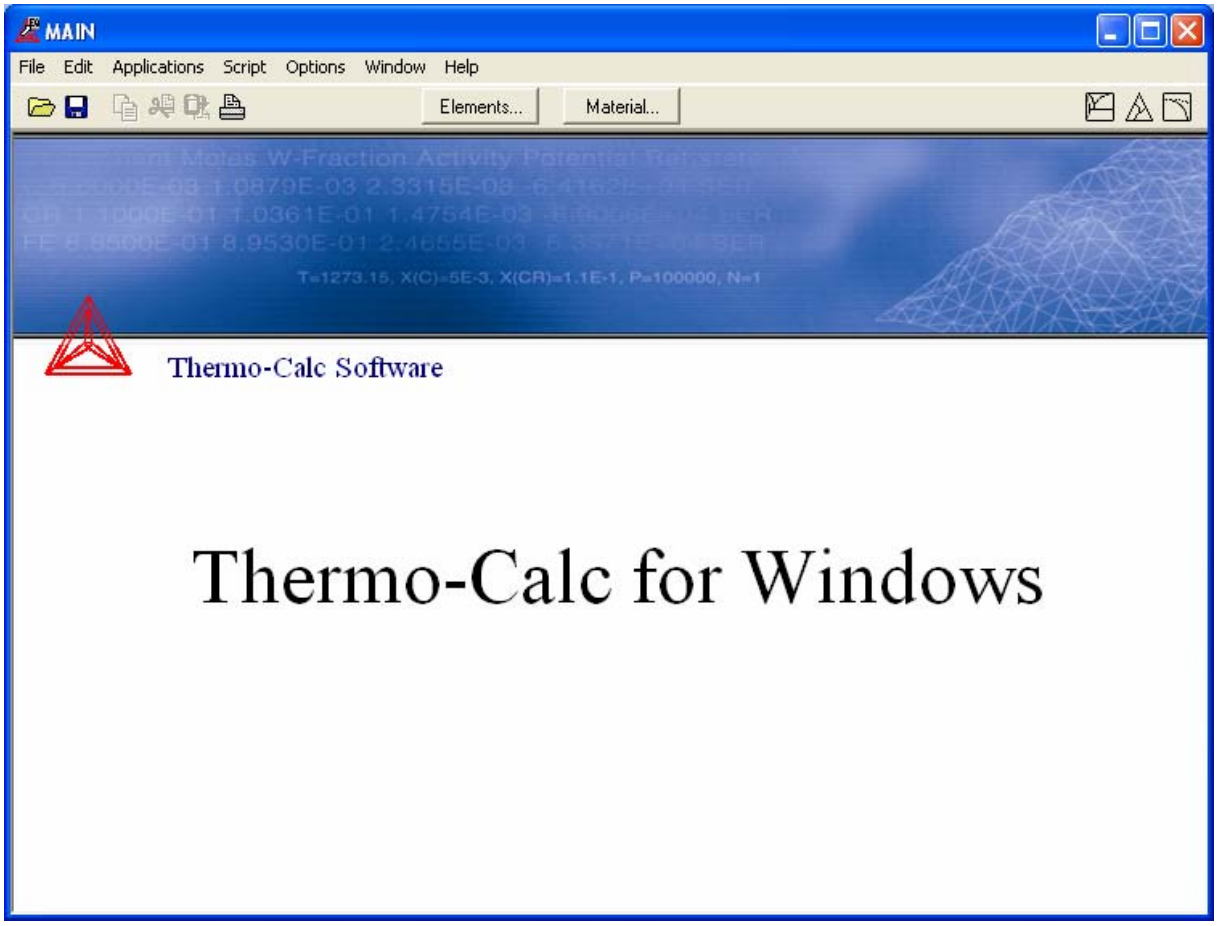
Acknowledgement of Copyright and Trademark Names:

CONTENT

1 Calculation of the Fe-Cr Phase Diagram

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

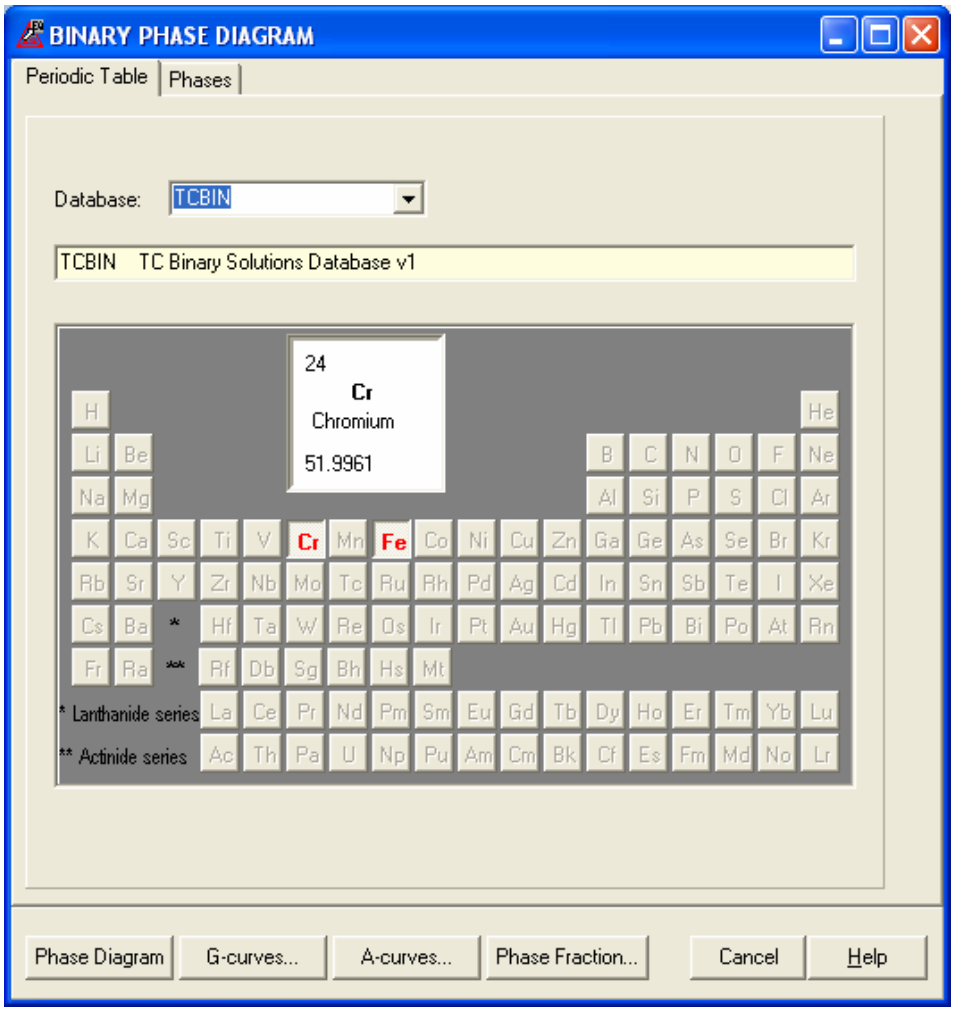
2. Click the  button.

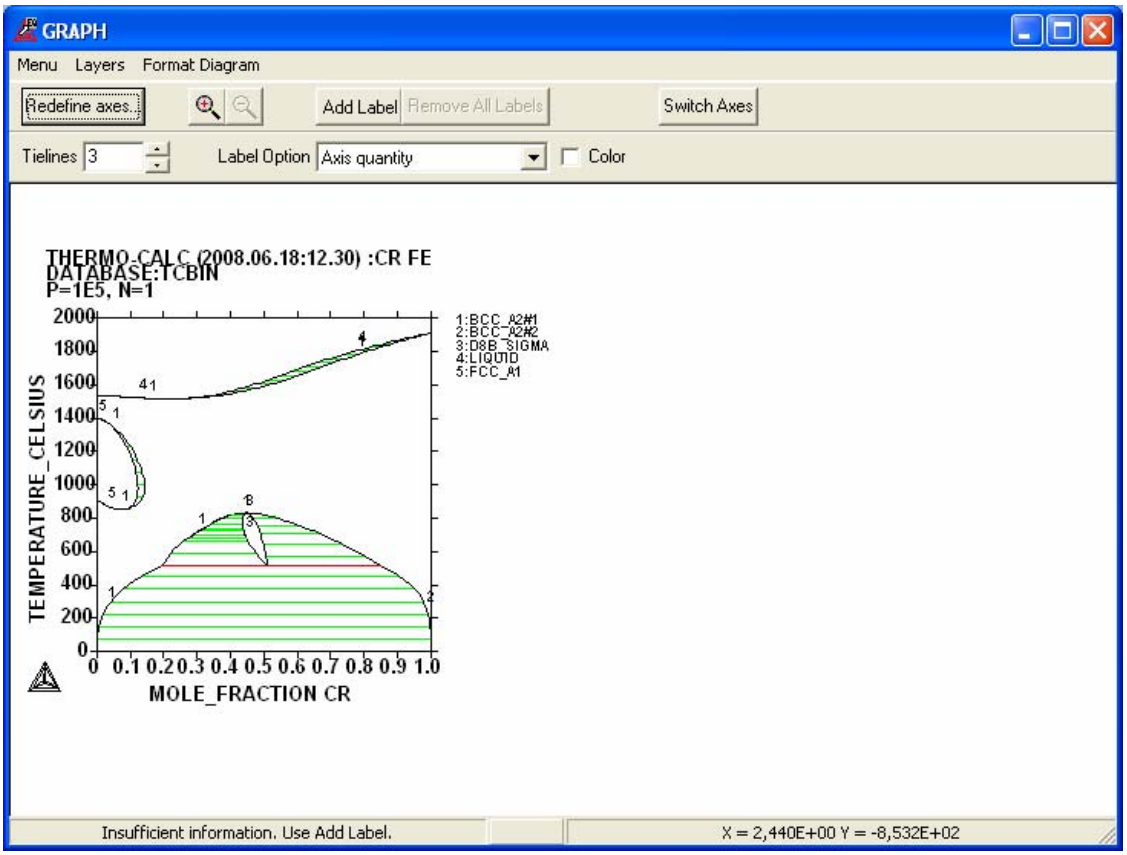


3. Select the elements *Fe* and *Cr* from the periodic table.

4. Click the *Phase Diagram* button.

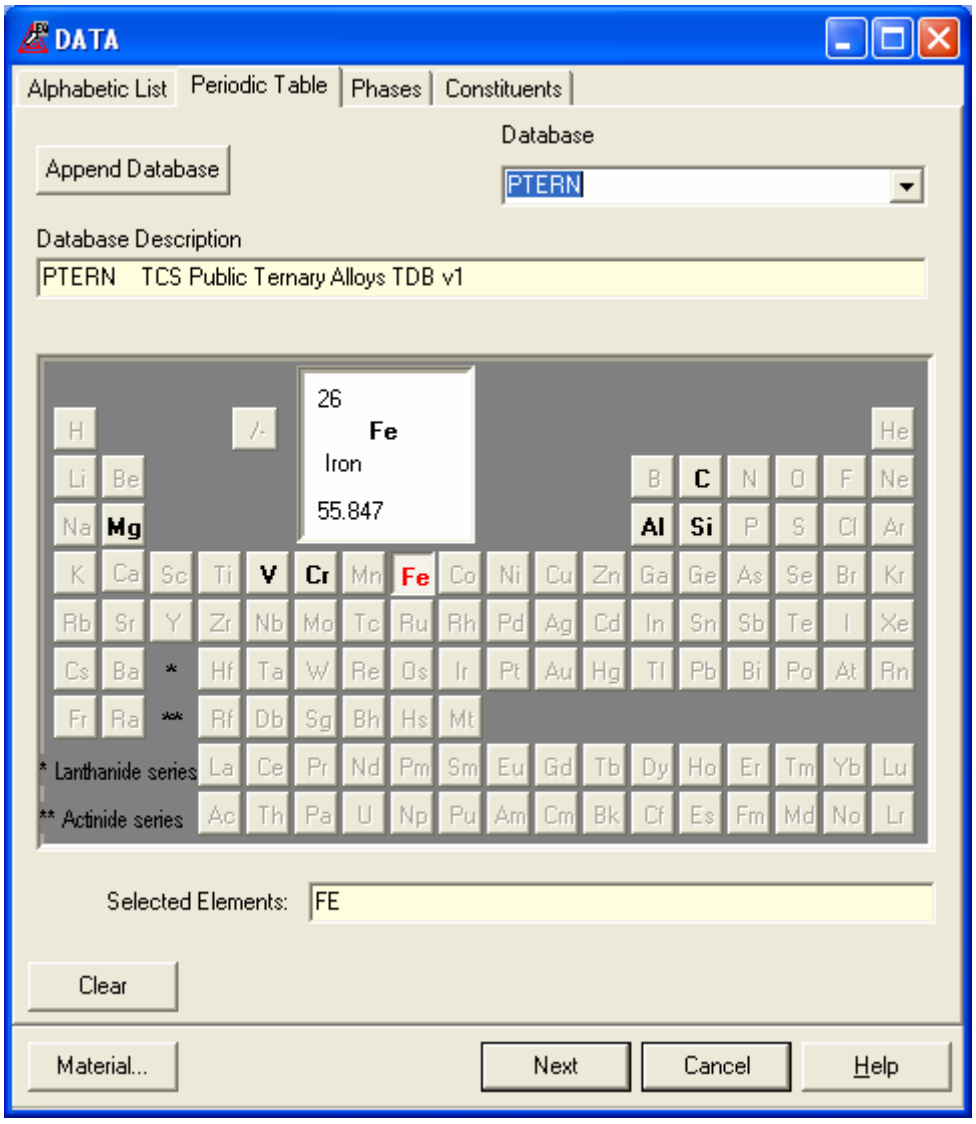
5. The Fe-Cr binary phase diagram will be calculated and plotted automatically.


BINARY PHASE DIAGRAM
Periodic Table
Phases
Database:
TCBIN
TCBIN TC Binary Solutions Database v1
24
Cr
Chromium
51.9961
* Lanthanide series
** Actinide series
Phase Diagram
G-curves...
A-curves...
Phase Fraction...
Cancel
Help

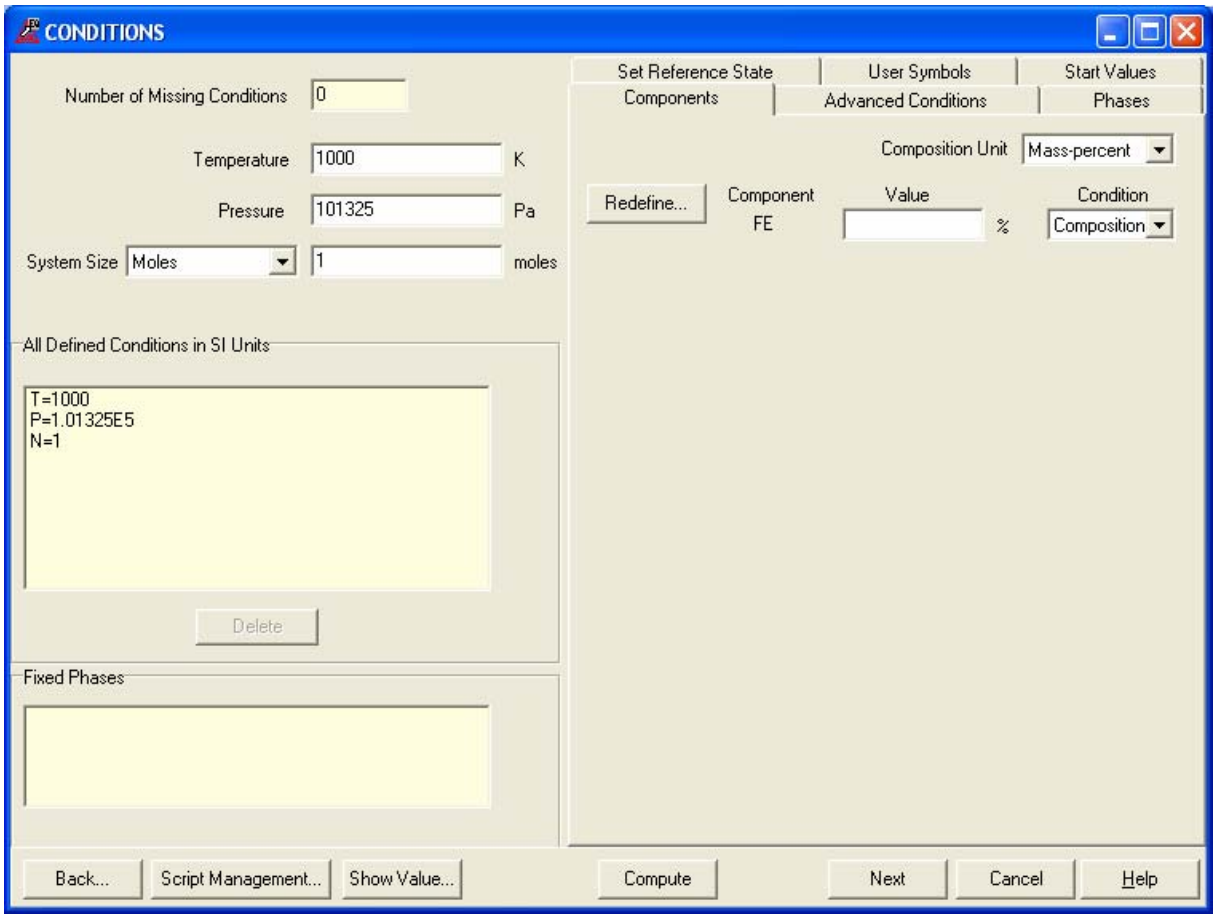

GRAPH
Menu
Layers
Format Diagram
Redefine axes...
Add Label
Remove All Labels
Switch Axes
Tielines
Label Option
Axis quantity
Color
THERMO-CALC (2008.06.18:12.30) :CR FE
DATABASE:TCBIN
P=1E5, N=1
1:BCC_A2#1
2:BCC_A2#2
3:D8B_SIGMA
4:LIQUID
5:FCC_A1
TEMPERATURE_CELSIUS
MOLE_FRACTION CR
Insufficient information. Use Add Label.
X = 2,440E+00 Y = -8,532E+02

2 Plotting Thermodynamic Functions

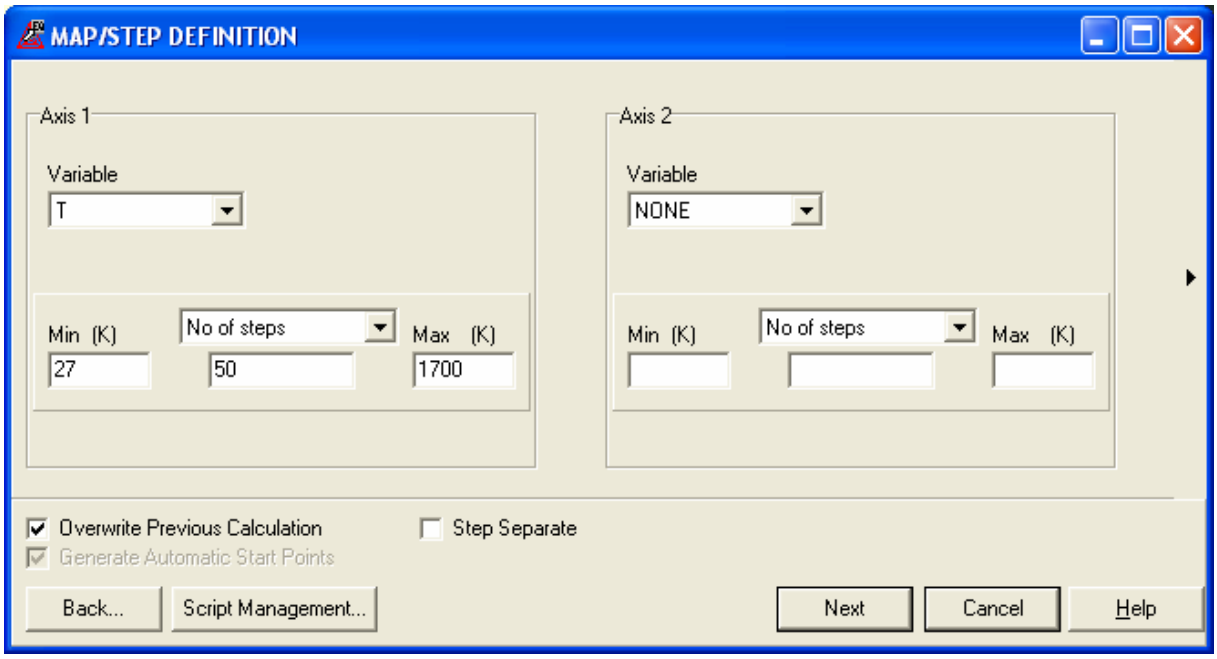
1. Choose the *Elements* button in the MAIN window. Select *Fe* from the *PTERN* database. Press *Next*.



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



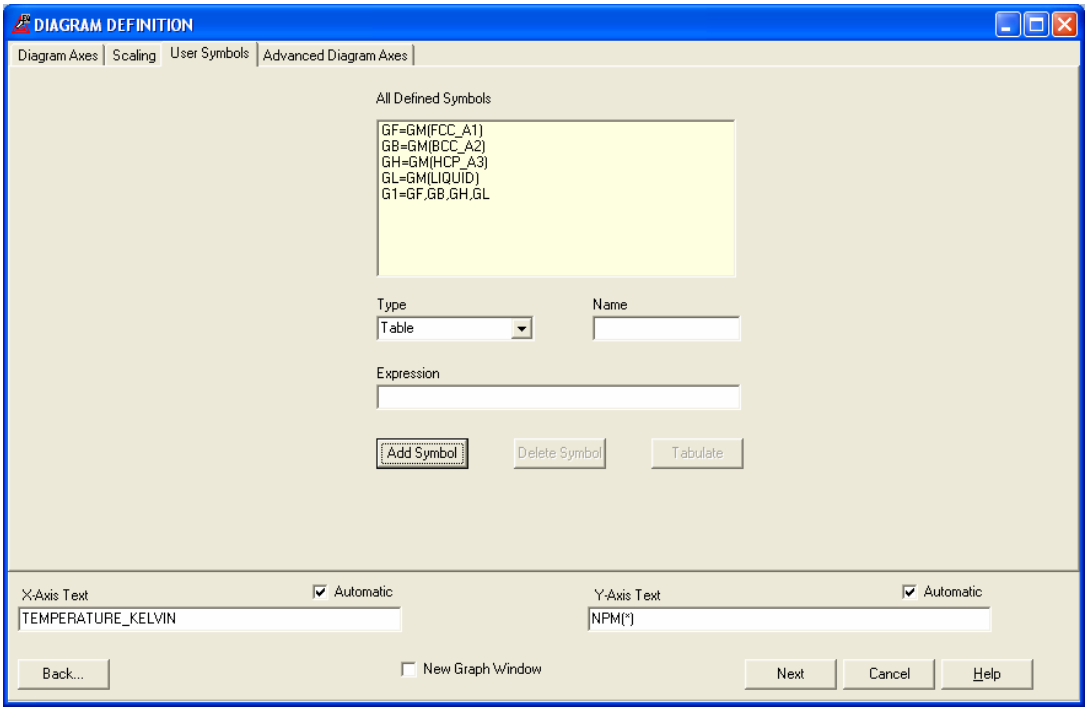
3. Define axis 1 as *T* and axis 2 as *NONE*. Enter min and max values as 27 resp. 1700 K. (The default temperature unit can be changed in the *Options* menu in the MAIN window.) Click *Next* to start the stepping.



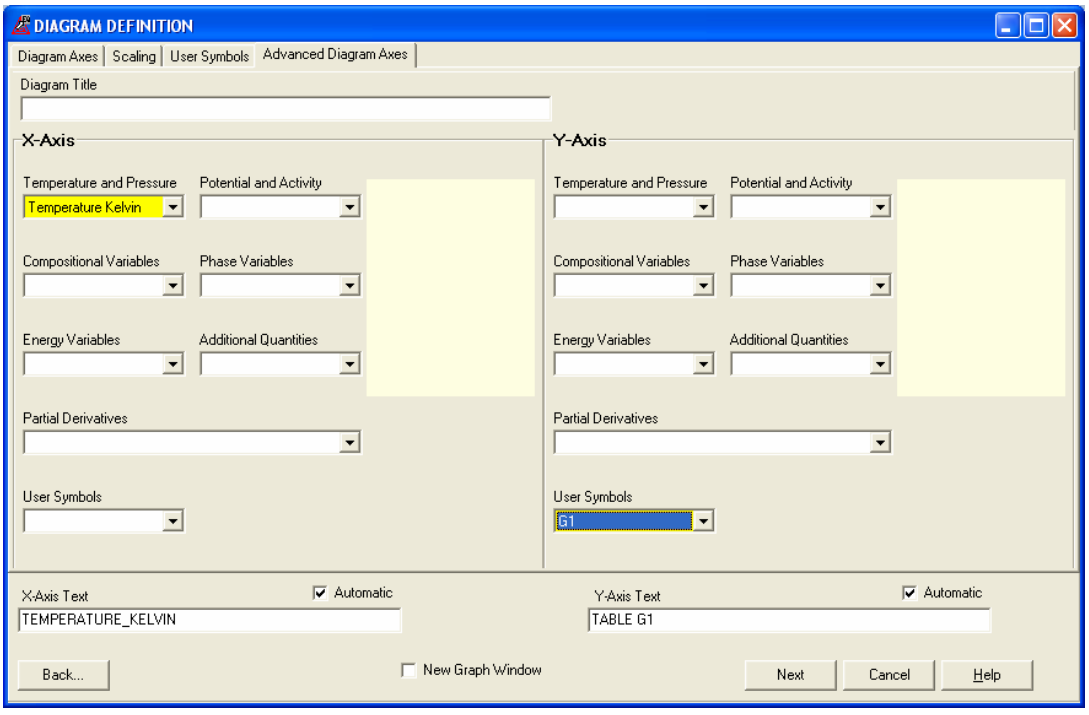
4. In order to plot thermodynamic functions for the individual phases, select the *User Symbols* tab in the DIAGRAM window and type in following four functions and one table, using the *Type*, *Name* and *Expression* boxes. Click *Add Symbol* after each definition.

Function GF=GM(FCC)
GB=GM(BCC)
GH=GM(HCP)
GL=GM(LIQUID)

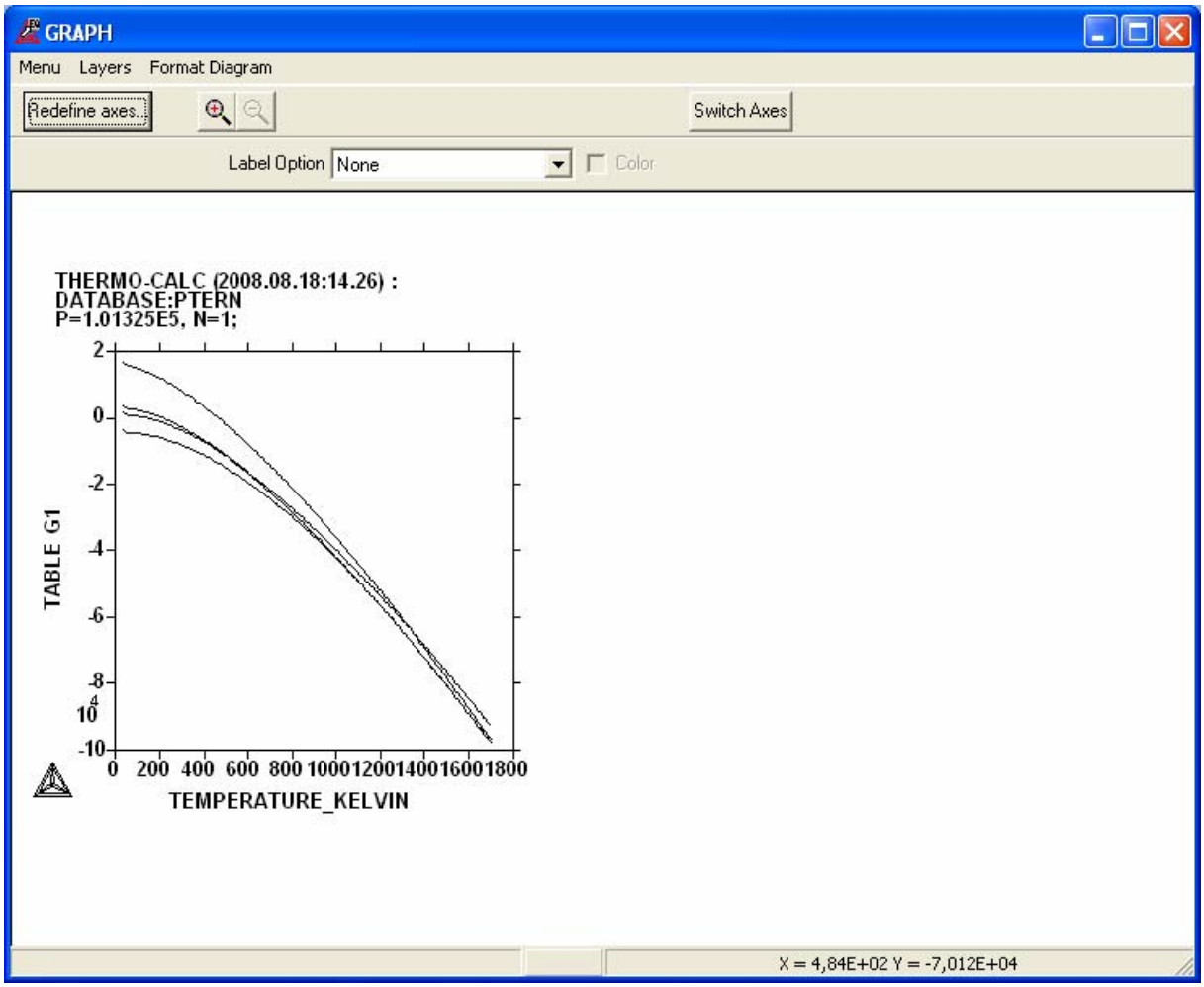
Table G1=GF,GB,GH,GL



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.



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

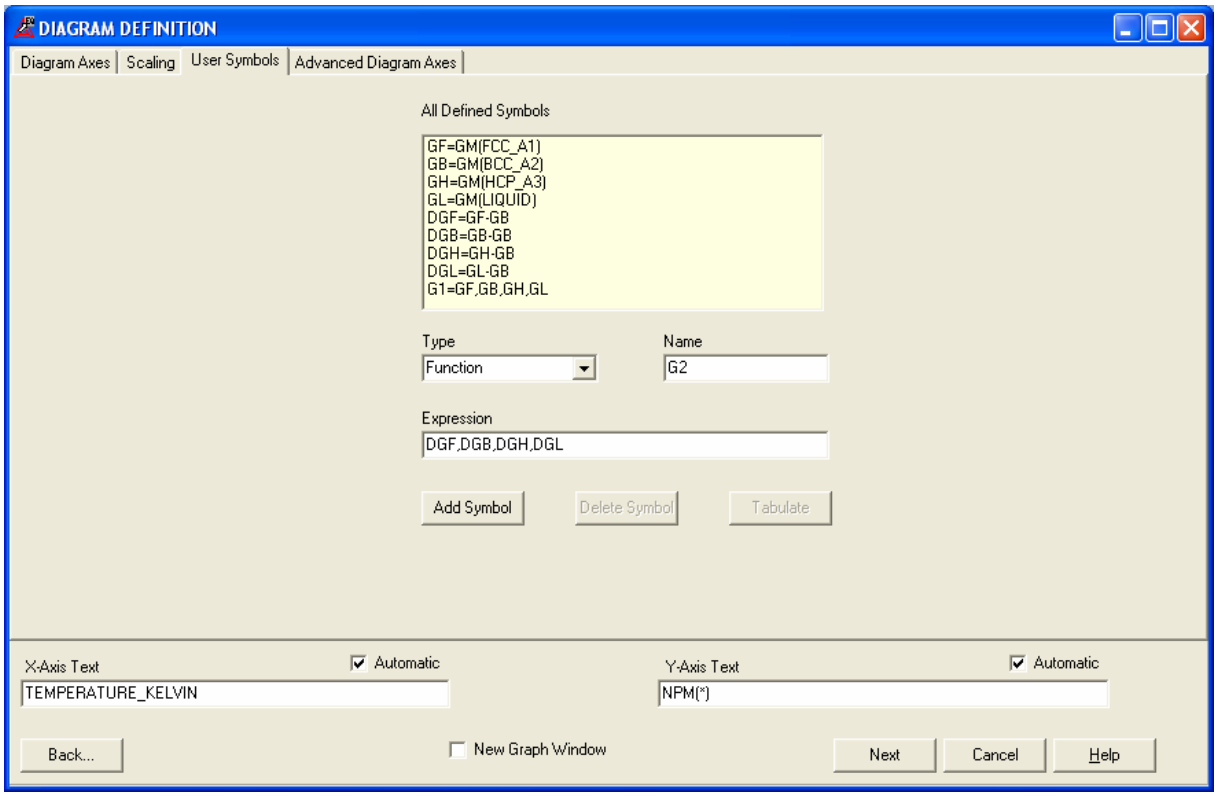


7. Type in new functions *DGF*, *DGH*, *DGL* which are the difference between the Gibbs energy for each phase compared with the Gibbs energy of the BCC phase. *DGB* will naturally be zero. Enter the functions in a table *G2*.

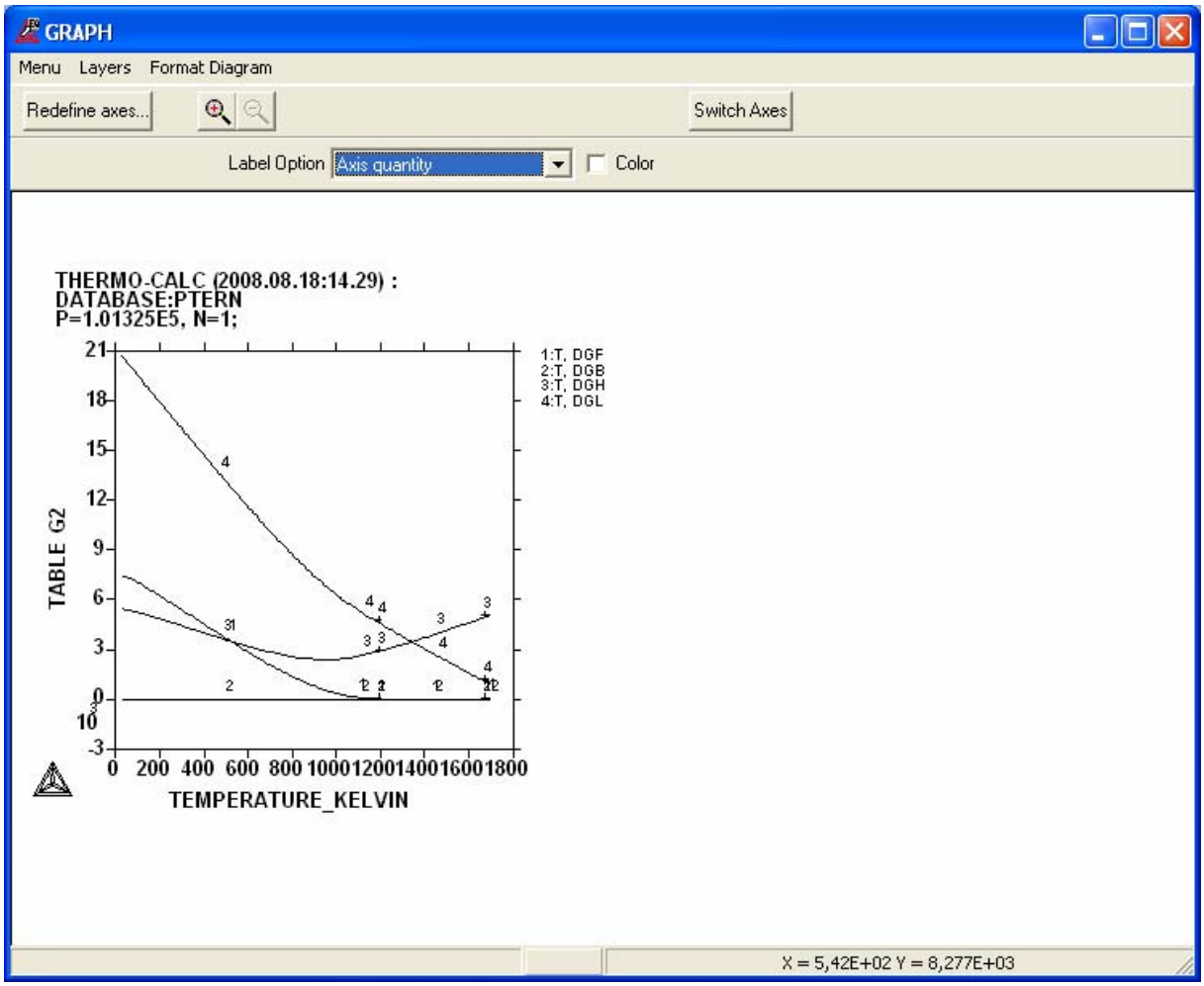
Function DGF=GF-GB
DGB=GB-GB
DGH=GH-GB
DGL=GL-GB

Table G2=DGF,DGB,DGH,DGL

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



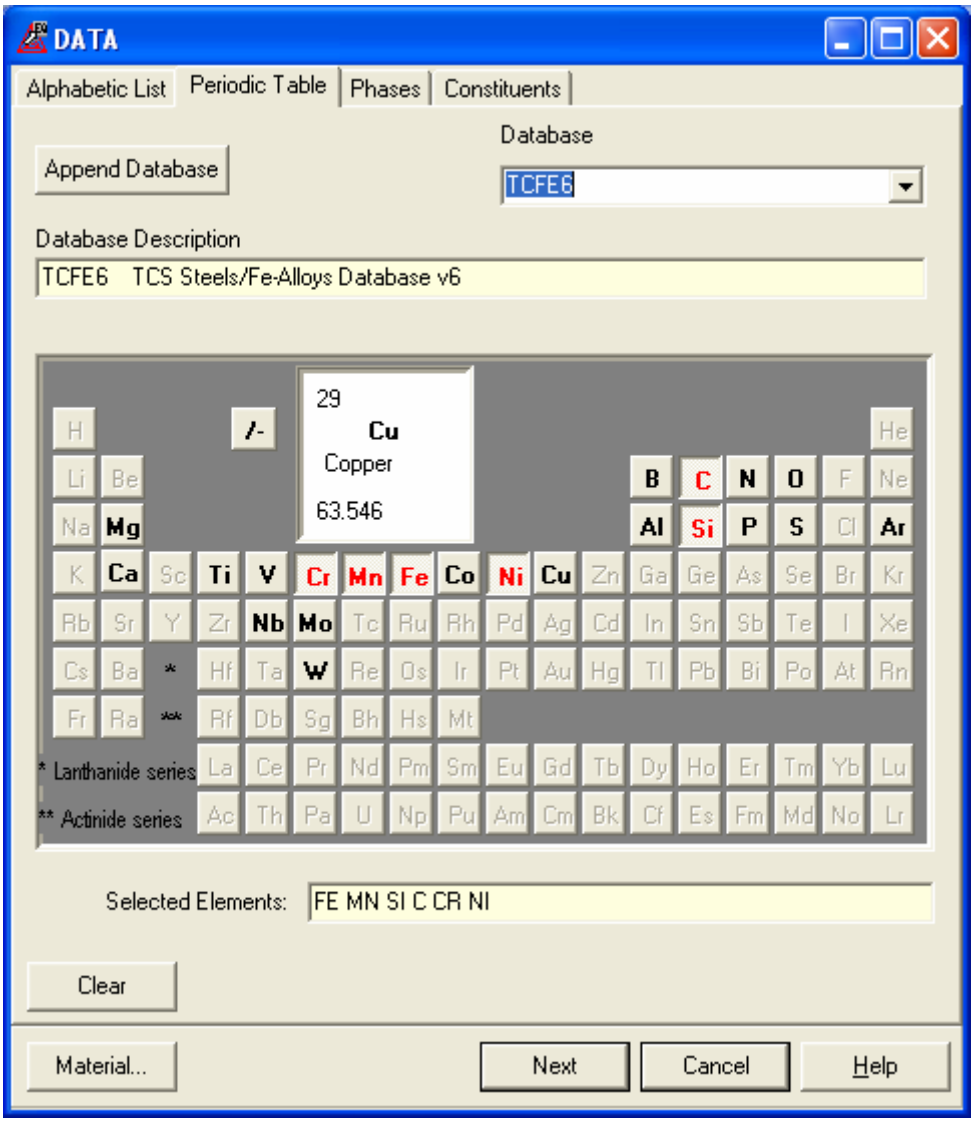
8. Select *Axis quantity* from the *Label Option* list.


GRAPH
Menu Layers Format Diagram
Redefine axes...
Switch Axes
Label Option
Axis quantity
Color
THERMO-CALC (2008.08.18:14.29) :
DATABASE:PTERN
P=1.01325E5, N=1;
1:T, DGF
2:T, DGB
3:T, DGH
4:T, DGL
TABLE G2
TEMPERATURE_KELVIN
X = 5,42E+02 Y = 8,277E+03

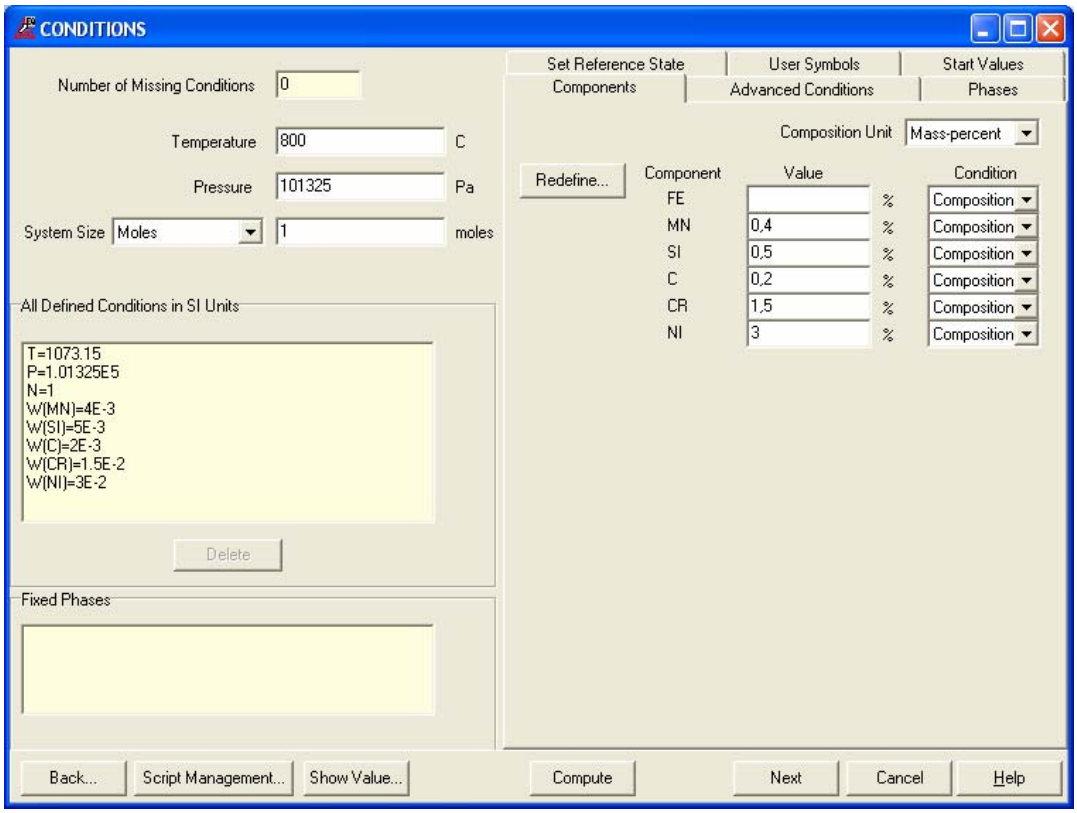
3 Calculation of Single Equilibrium in Low Alloyed Fe-Mn-Si-Cr-Ni-C Steel

1. Start TCW and click *Elements* on the MAIN window.

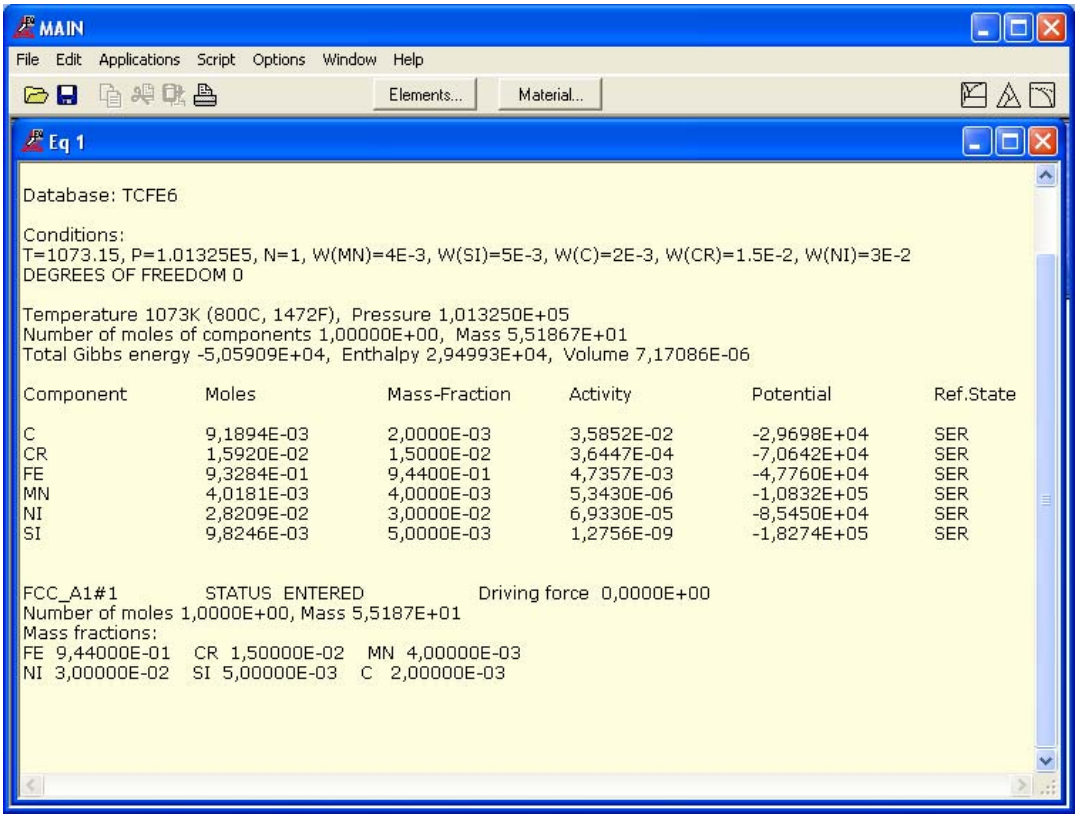
2. In the DATA window, choose the *TCFE6* database and select the following six elements; Fe, Mn, Si, C, Cr, Ni. Finish by clicking *Next*.



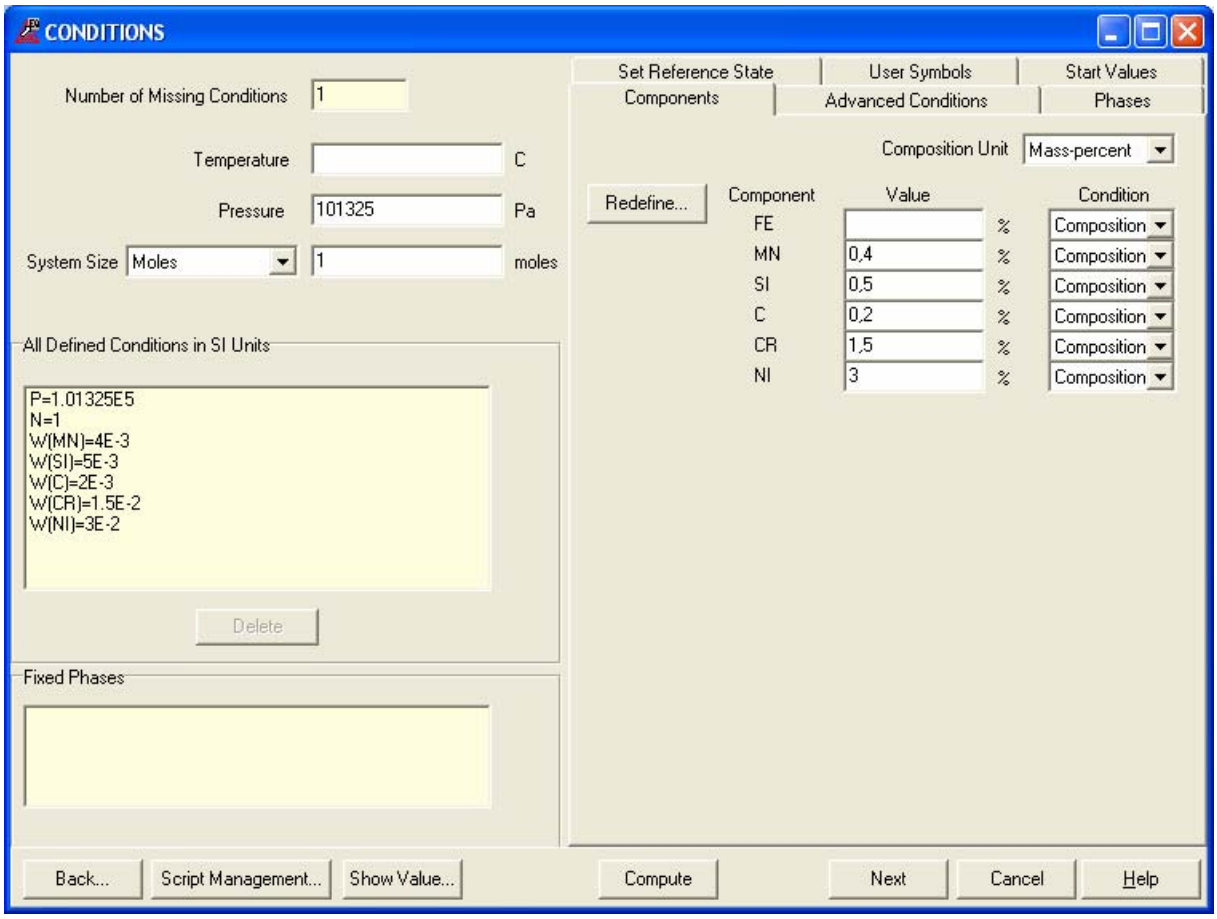
3. To do an equilibrium calculation at 800 °C, enter this temperature in the *Temperature* box. (The default temperature unit can be changed in the *Options* menu in the MAIN window). Then enter the composition values in mass-percent for all the elements except the major Fe in the boxes on the right 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.



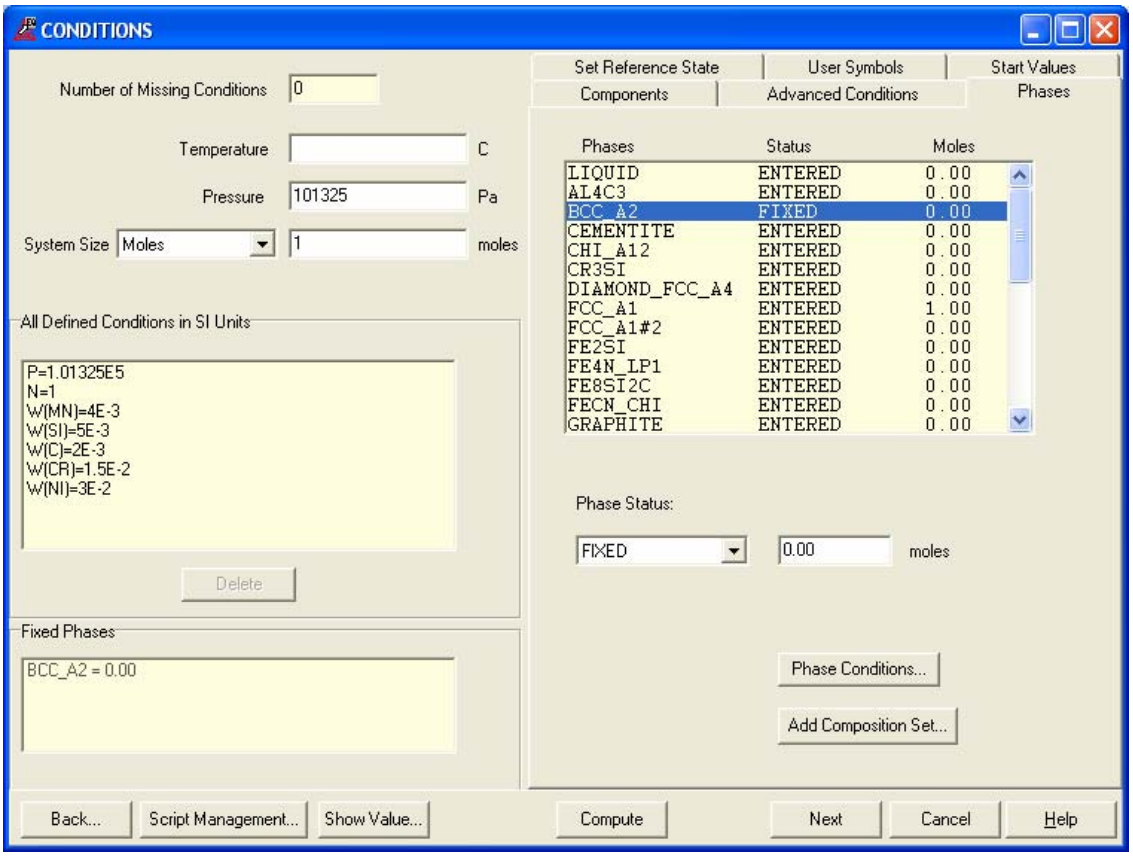
4. The result of this calculation is now shown in the MAIN window. The listing is equivalent to the output from the LIST-EQUILIBRIUM command in Thermo-Calc Classic. Under the present conditions, only fcc phase (austenite) is present as a stable phase. Note that the CONDITIONS window is still open for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



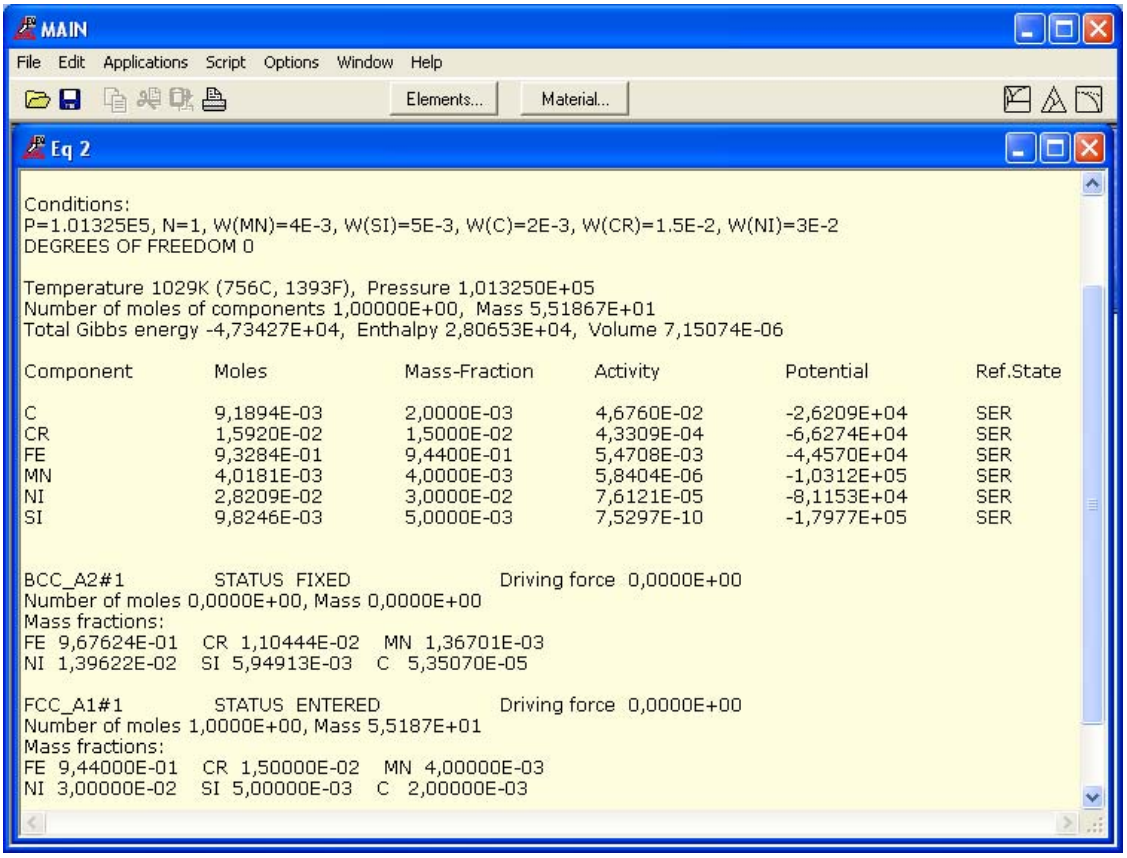
5. A more interesting calculation is to find out at what temperature bcc (ferrite) becomes stable for this steel (the A3 line). Go back to the CONDITIONS window and take away the condition on temperature (mark *T=800* in the list and click *Delete*, or clear the *Temperature* box). The degrees of freedom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



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*.



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 ºC.

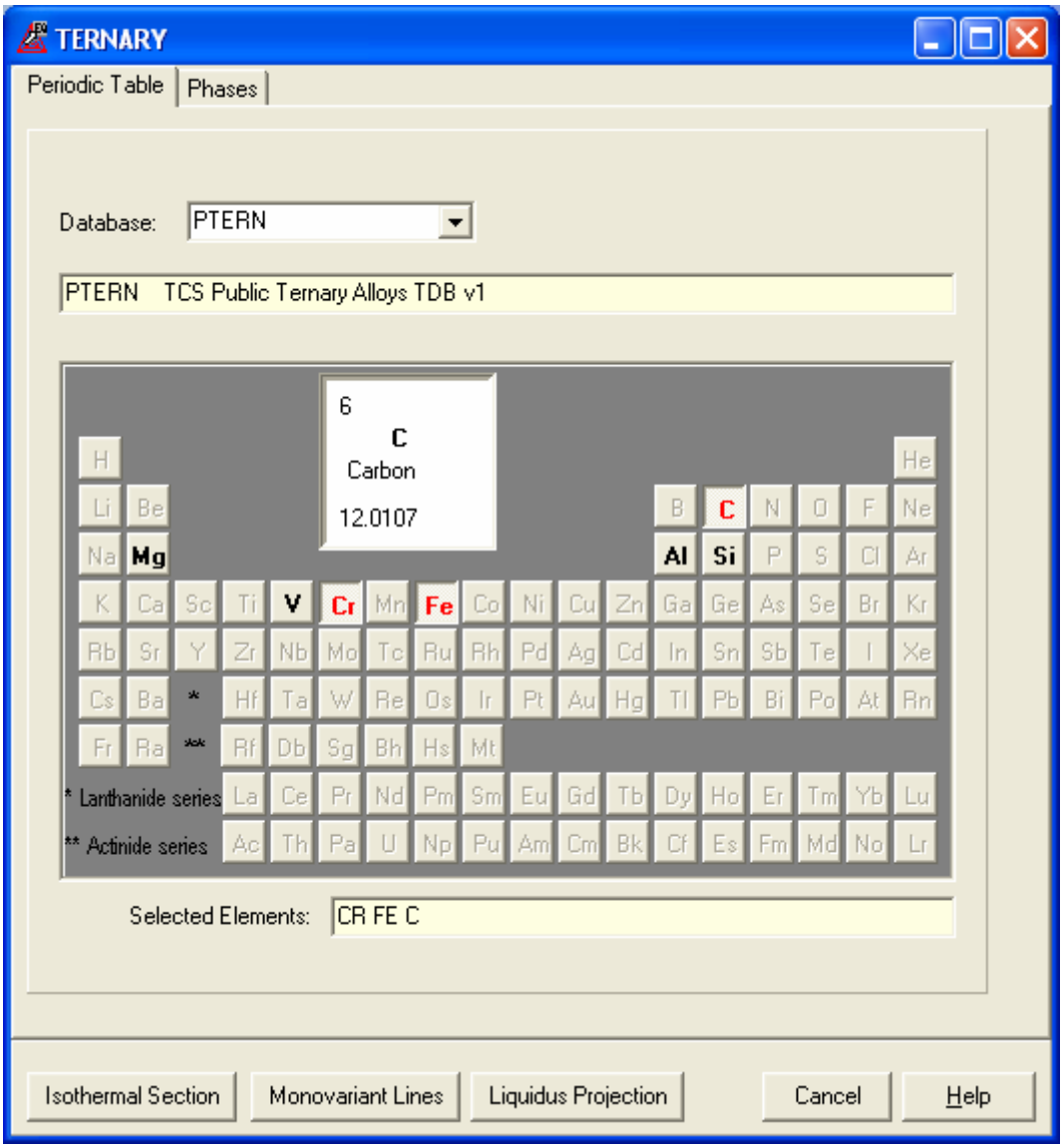


4 Isothermal Section of the Fe-Cr-C System at 1000 K

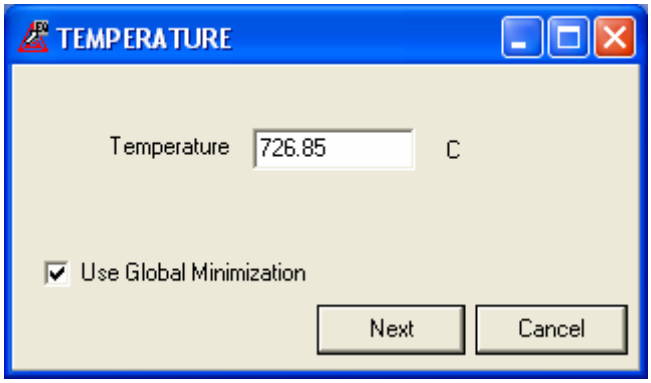
1. Here we use the ternary module in TCW, which is opened by clicking 

2. Select the *PTERN* database in the *Database* box and click the three elements in the periodic table; Cr, Fe, and C.

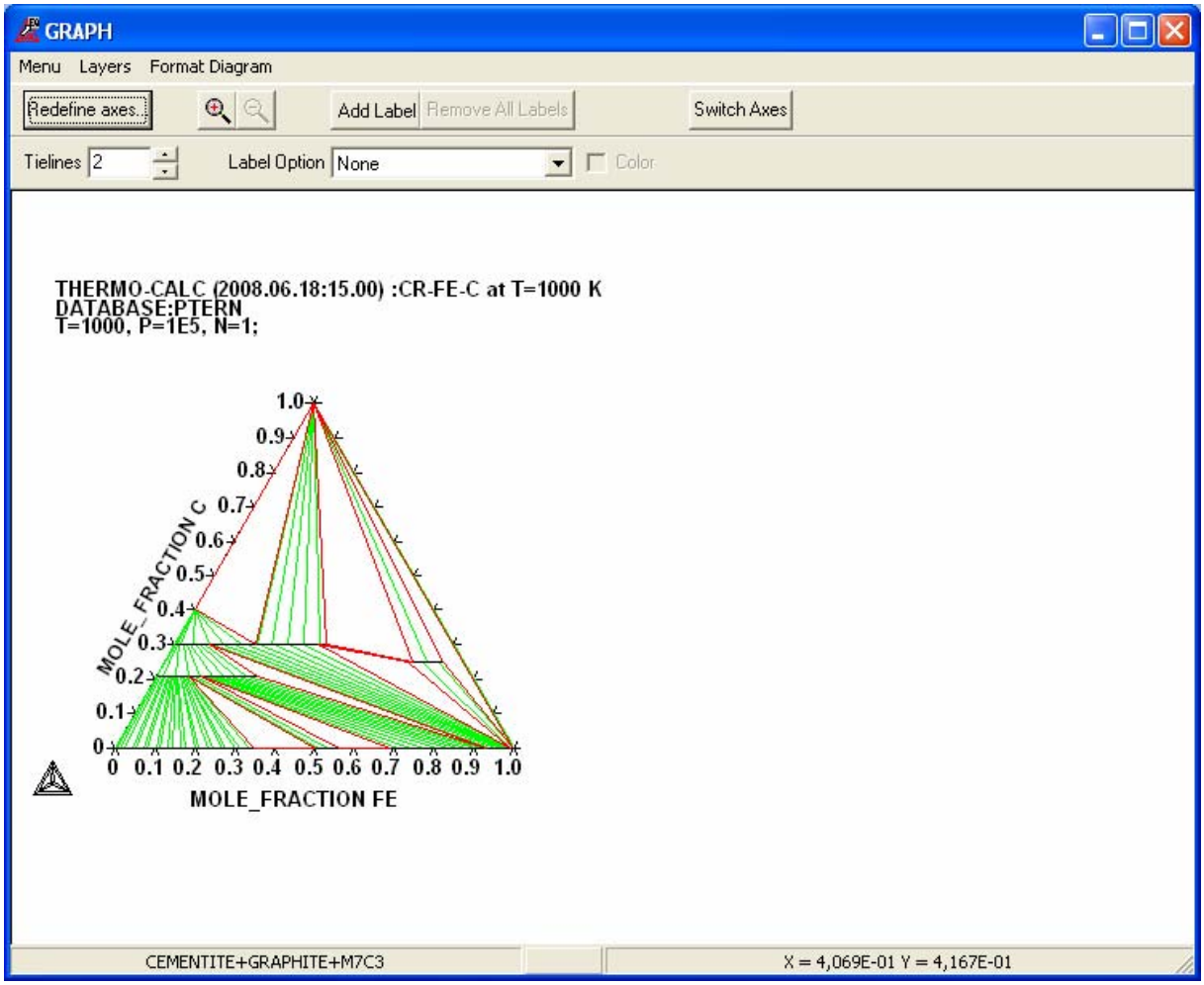
3. Click *Isothermal Section* to continue.



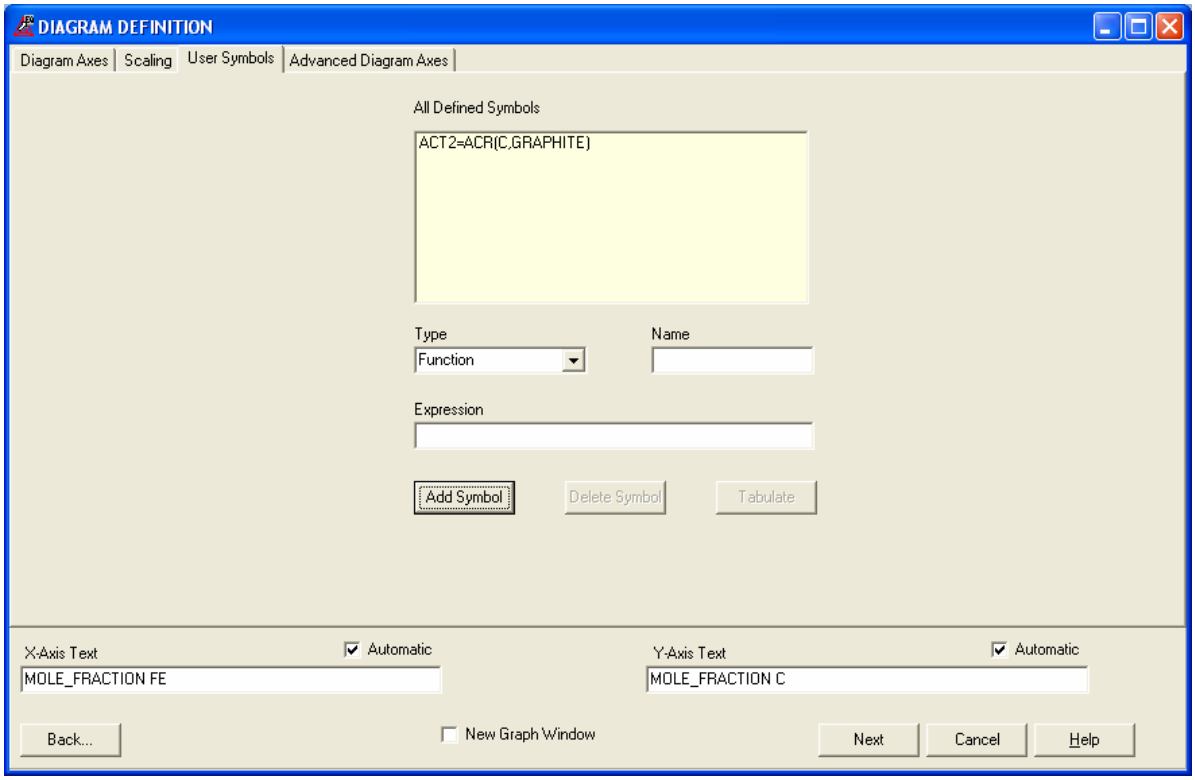
4. When the temperature box appears the temperature is set to 726.85 ºC (1000 K). The default unit may be changed to K in the *Options/Units* menu in the MAIN window. Click *Next* to proceed.



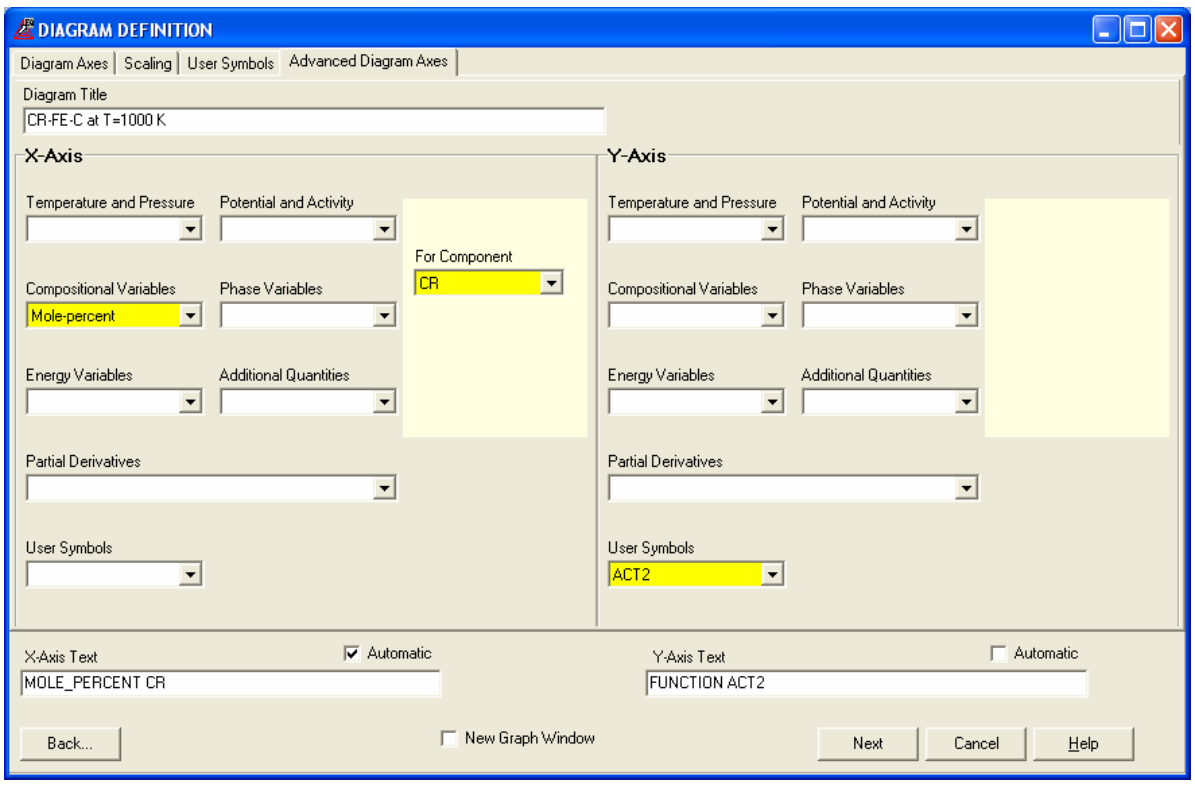
5. To plot the isothermal section click *next.* By placing the mouse cursor at a certain region in the diagram the name of the phase(s) stable in that region is displayed in the lower left corner of the GRAPH window.



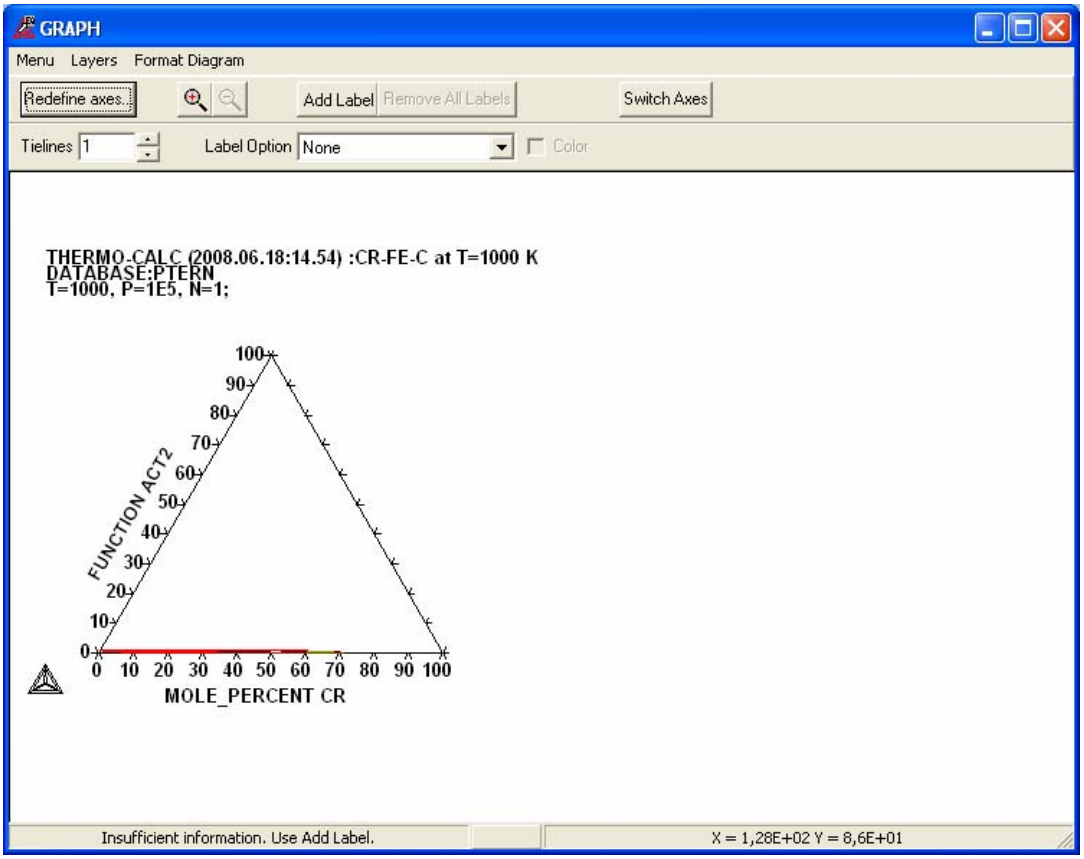
6. Press *Redefine* to plot amount of Cr vs. activity of carbon instead. To get easily understandable activity values, open the User Symbols tab and enter a function for the activity of carbon referred to the current temperature: ACT2=ACR(C,GRAPHITE).

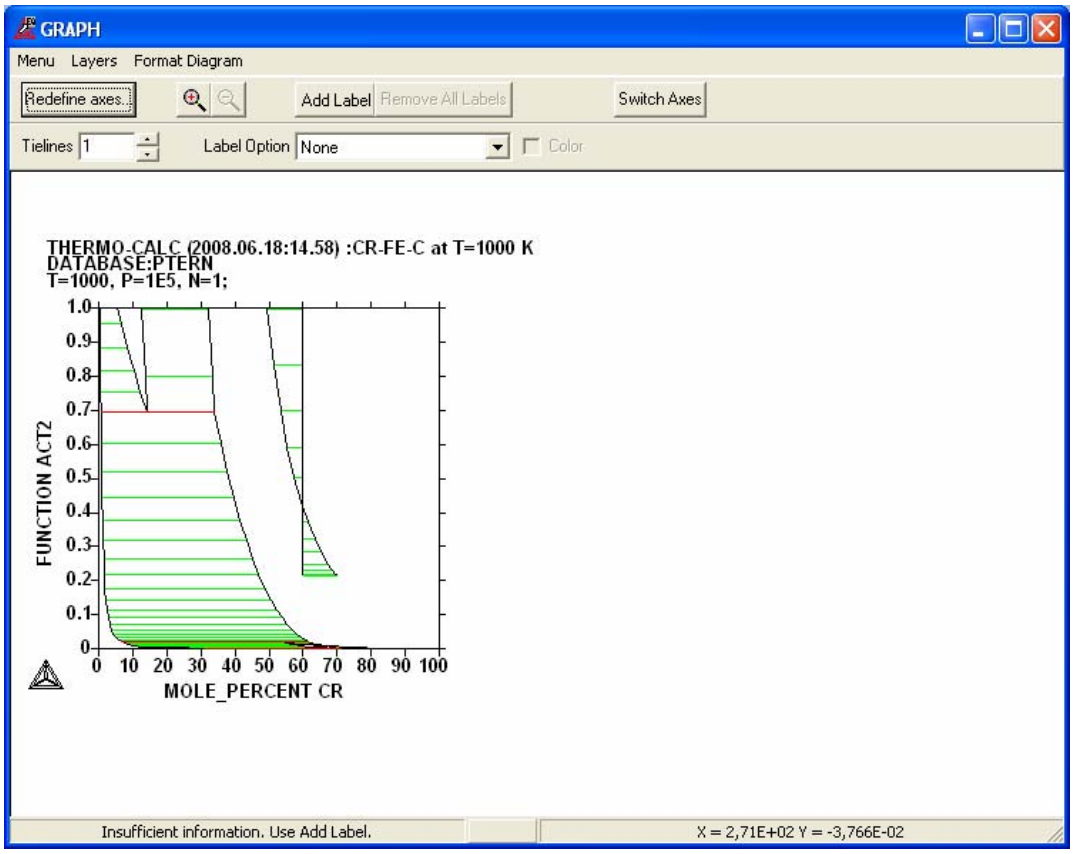


7. Next select *Advanced Diagram Axis* and set the X-Axis variable to Mass Percent Cr and the Y-Axis variable to the function ACT2. Click next to plot.



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





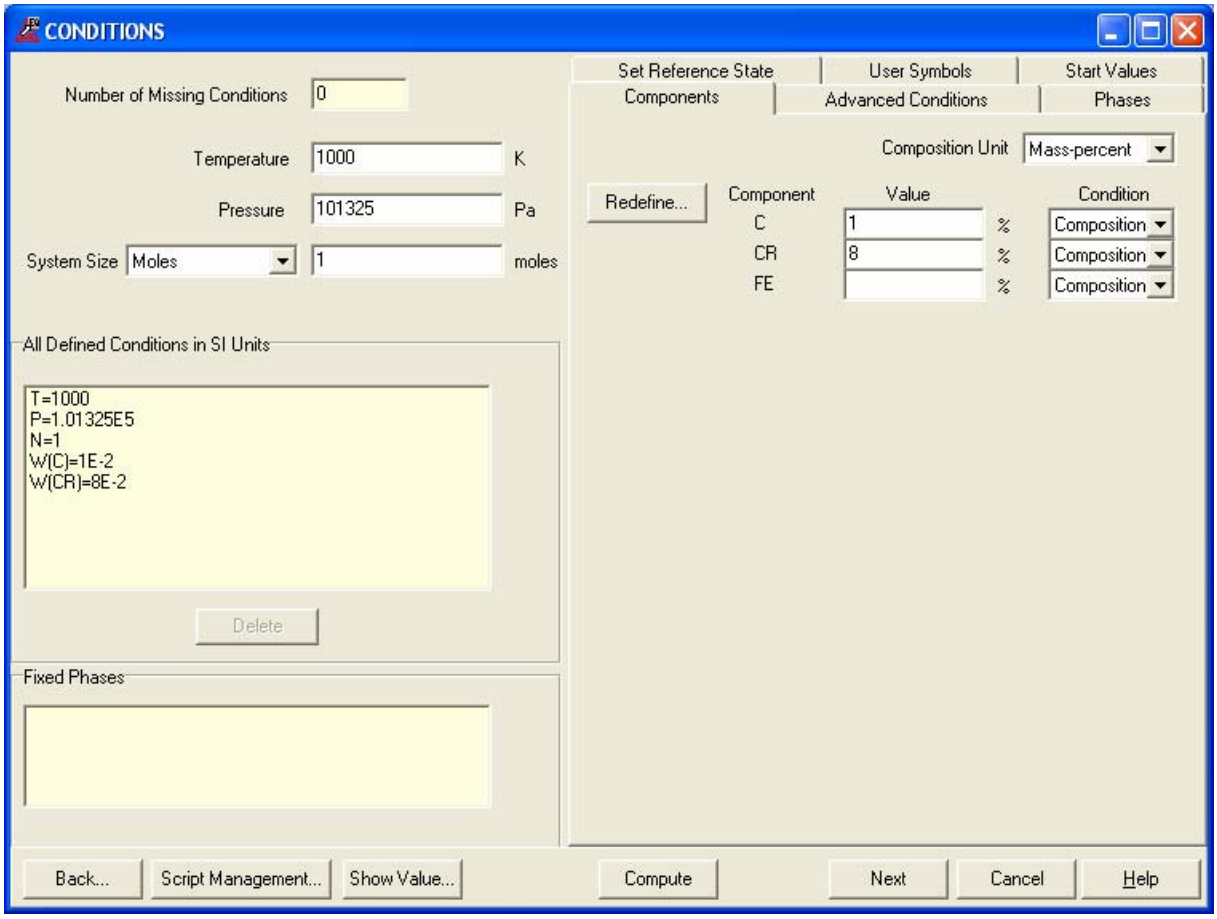
5 Calculation of Isopleth in Fe-8Cr-1C System

1. Open the TCW program.

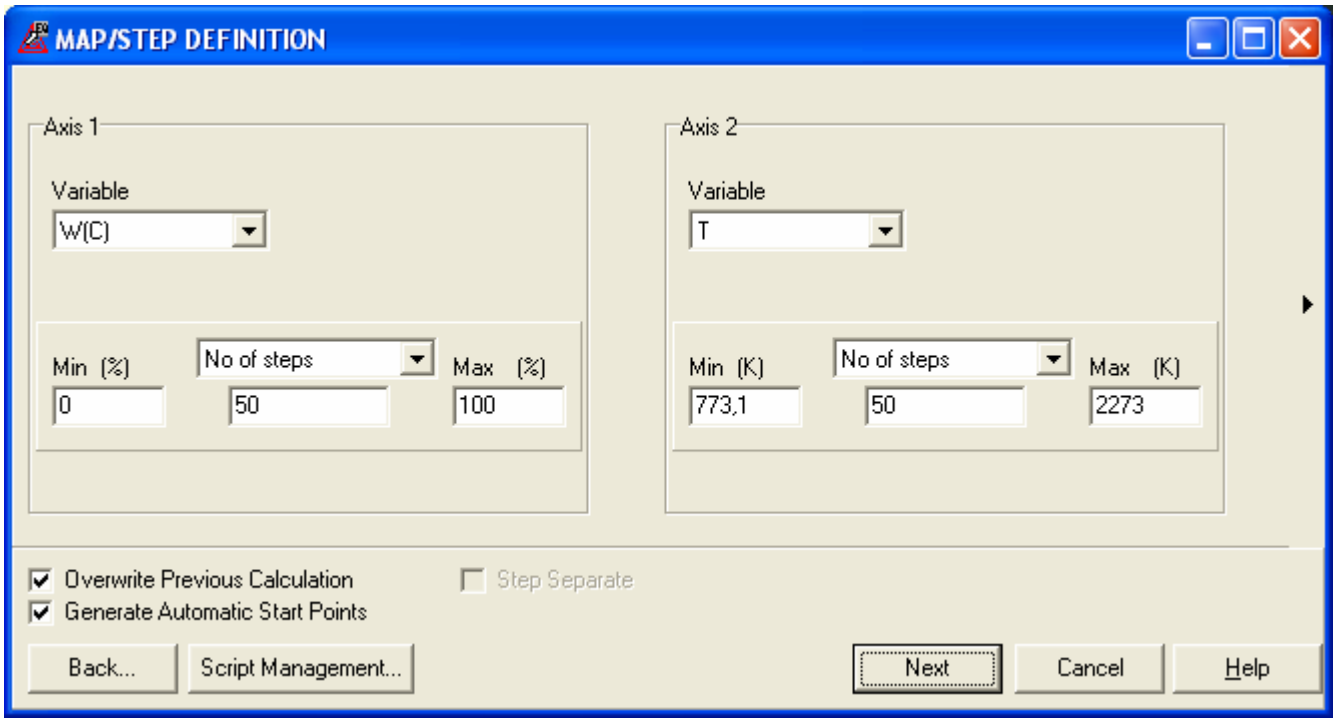
2. Click *Elements.*

3. Select *PTERN* from the *Database* list and then click alloy elements *C*, and *Cr, and Fe* in the periodic table. Click *Next*.

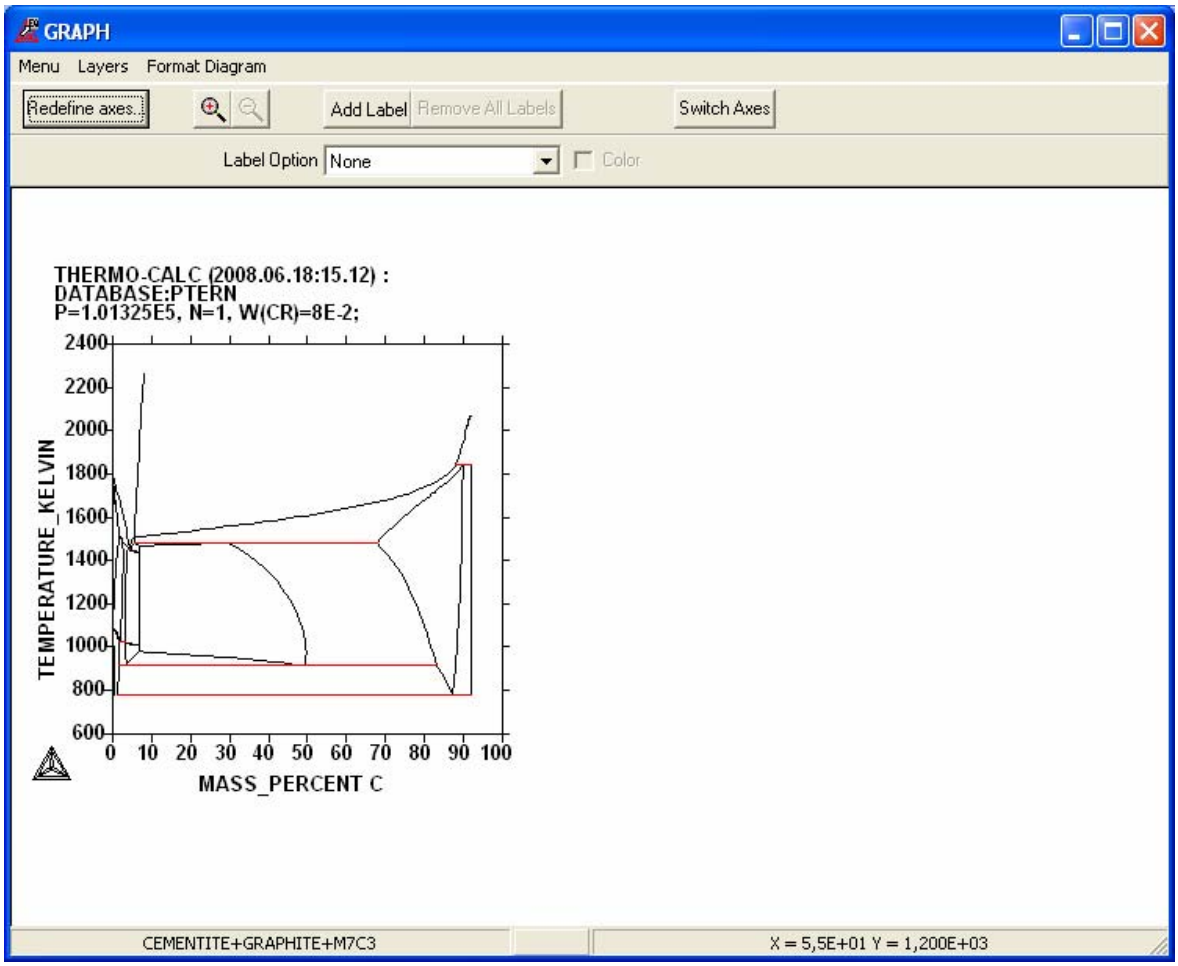
4. Specify the concentrations of C and Cr as *1* and *8 mass-percent*, respectively and accept the default temperature. Click *Next*.



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.*

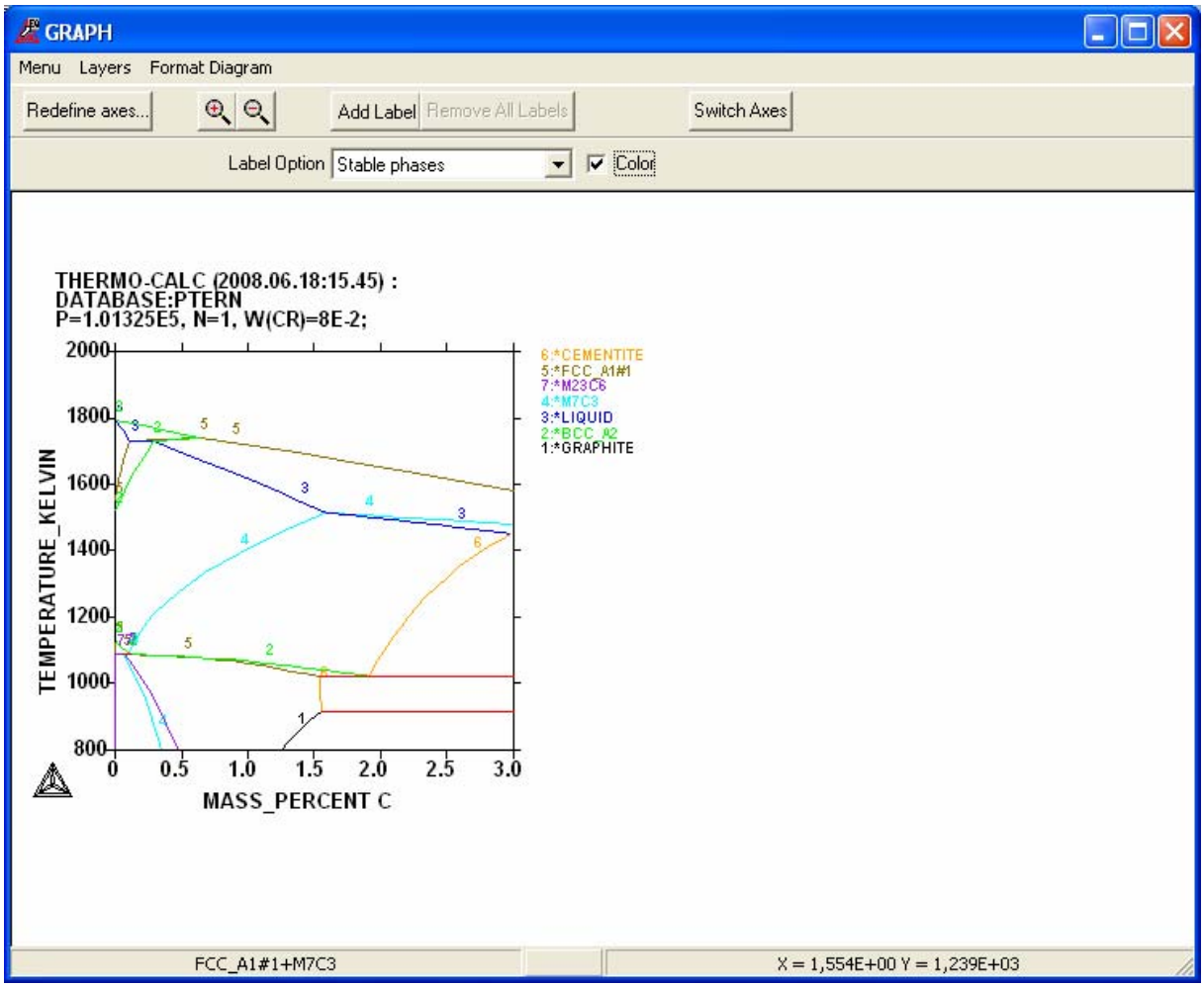


6. After the calculation is finished, the DIAGRAM DEFINITION window pops up. The mapping axes are shown as the default plotting X-axis and Y-axis now. Click *Next*. The following diagram is plotted.

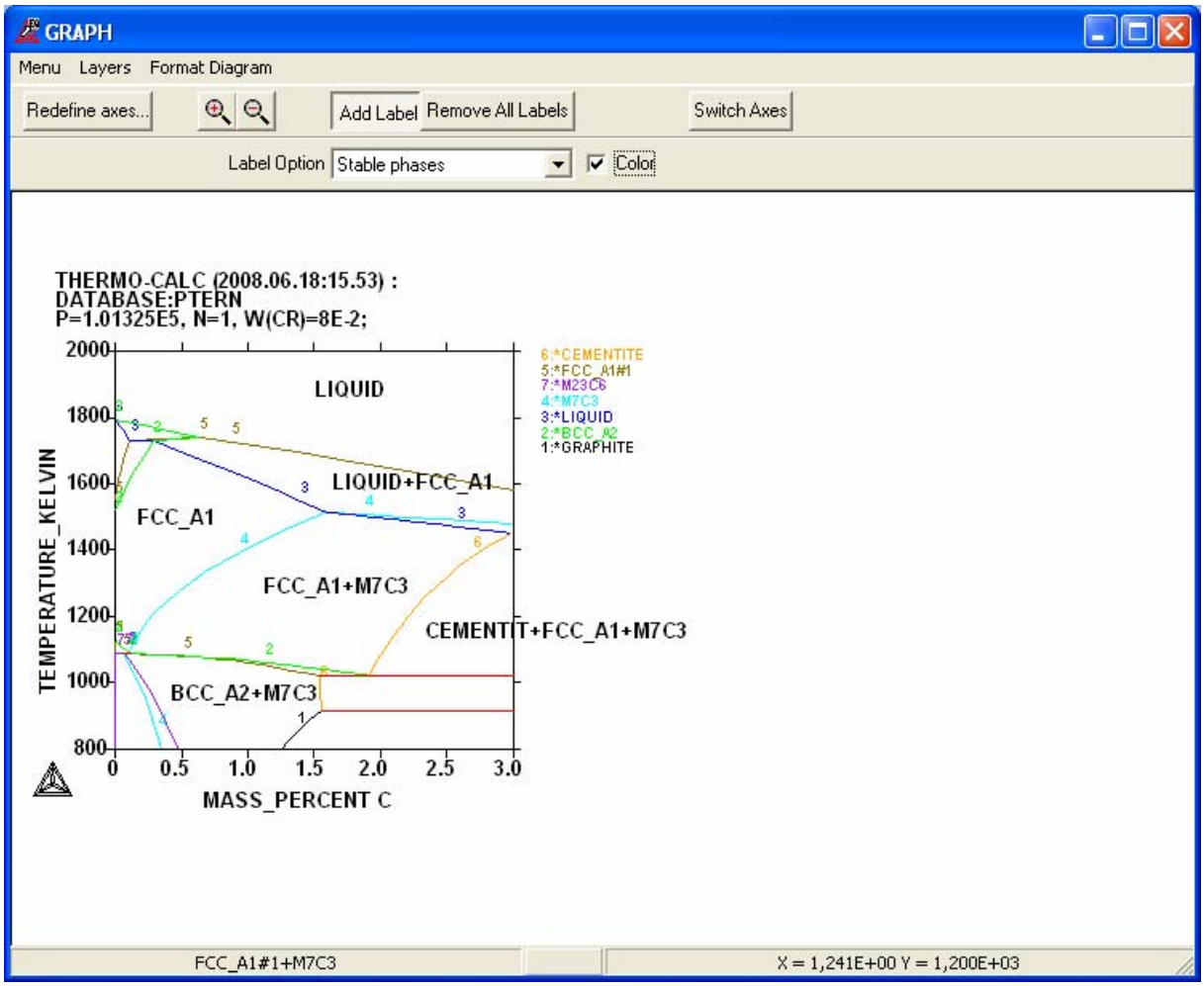


7. Choose *Scaling* from the *Format Diagram* menu to open the Scaling tab on the DIAGRAM DEFINITION window. Specify the min value for X-axis as *0* and max as *3*, and for Y-axis as *800* and *2000*. Click *Next*.

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.


GRAPH
Menu Layers Format Diagram
Redefine axes...
Add Label
Remove All Labels
Switch Axes
Label Option
Stable phases
Color
THERMO-CALC (2008.06.18:15.53) :
DATABASE:PTERN
P=1.01325E5, N=1, W(CR)=8E-2;
6:*CEMENTITE
5:*FCC_A1#1
7:*M23C6
4:*M7C3
3:*LIQUID
2:*BCC_A2
1:*GRAPHITE
LIQUID
LIQUID+FCC_A1
FCC_A1
FCC_A1+M7C3
CEMENTIT+FCC_A1+M7C3
BCC_A2+M7C3
TEMPERATURE_KELVIN
MASS_PERCENT C
2000
1800
1600
1400
1200
1000
800
0
0.5
1.0
1.5
2.0
2.5
3.0
FCC_A1#1+M7C3
X = 1,241E+00 Y = 1,200E+03

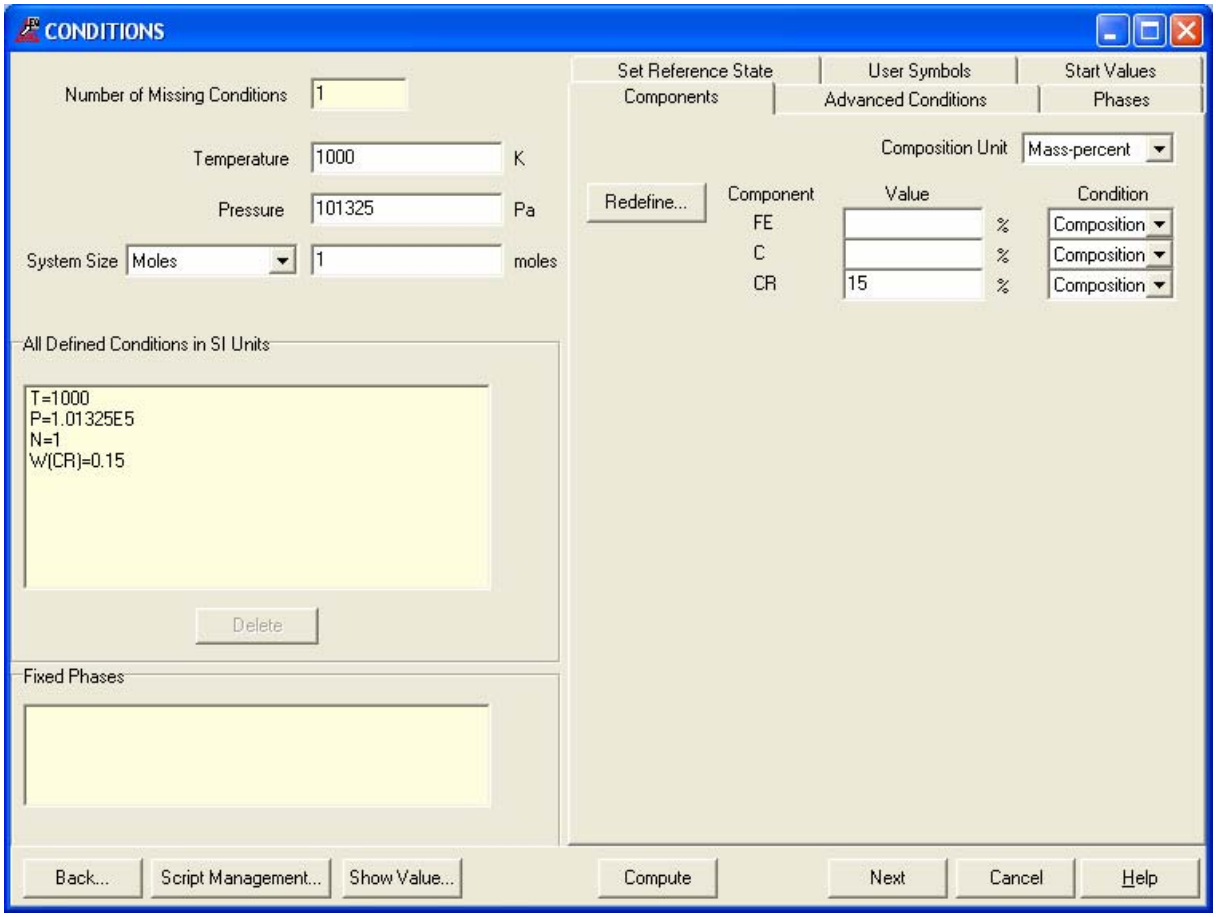
6 Calculation of a Vertical Section for Mixing of Fe-1Cr-0.1C and Fe-20Cr-2C Alloys

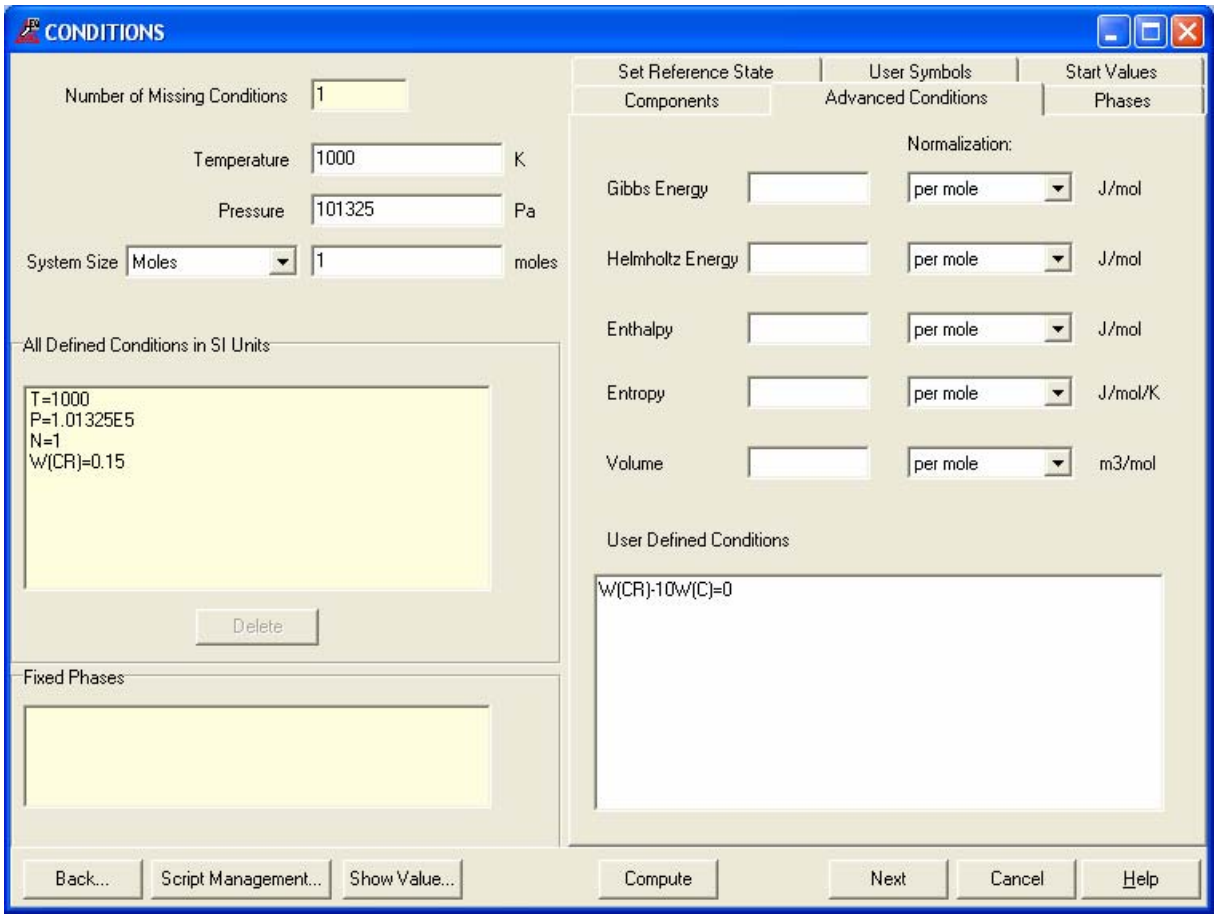
1. Open the TCW program.

2. Click *Elements.*

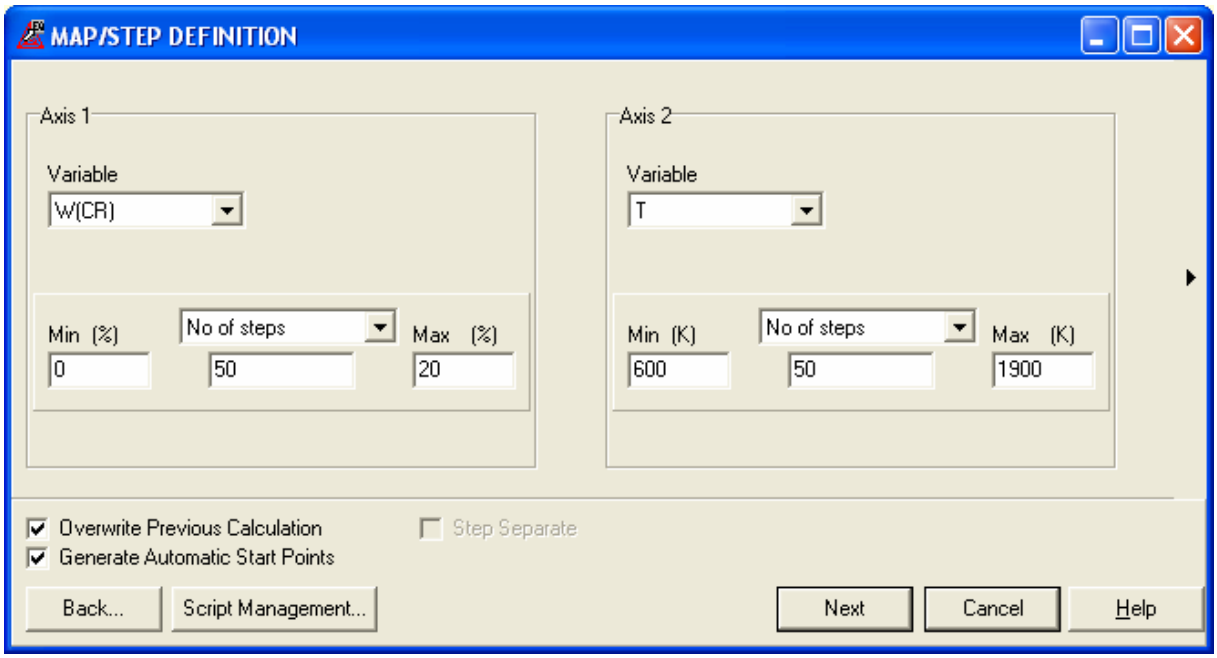
3. Select *PTERN* from the *Database* list and then click alloy elements *Fe*, *C*, and *Cr* in the periodic table. Click *Next*.

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(CR)/W(C)=(20-1)/(2-0.1)=19/1.9=10, i.e. W(CR)-10W(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(CR)-10W(C)=0* in the *User Defined Conditions* box. Click *Next*.

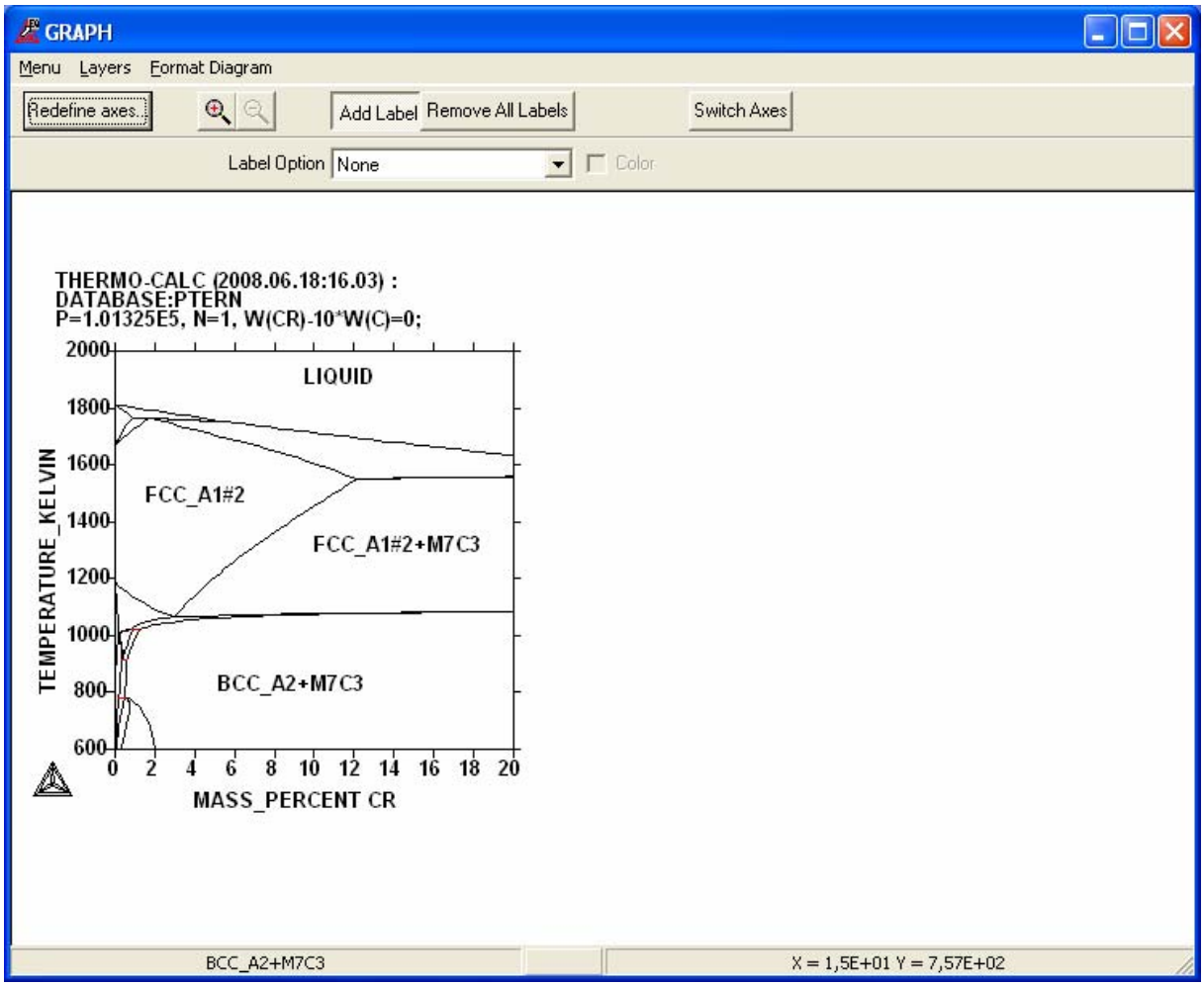




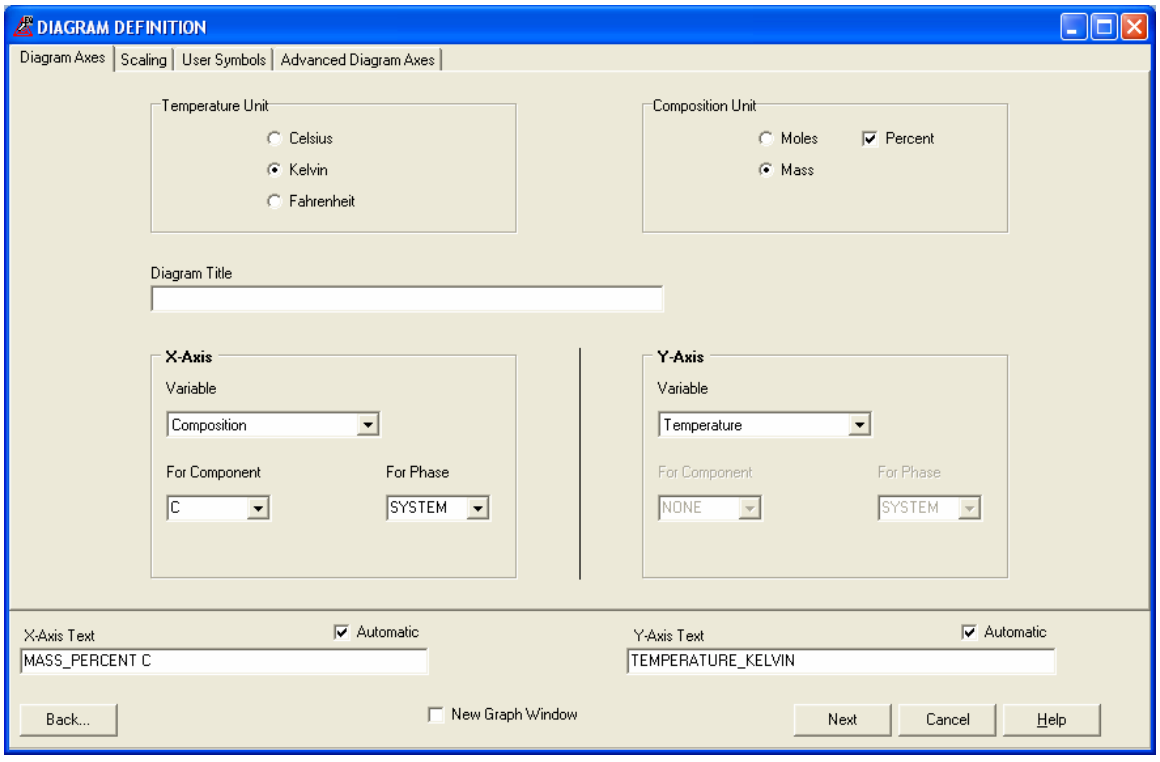
5. Define the mapping ranges: from 0 to 20%Cr and 600 to 1900 K. Click *Next*.



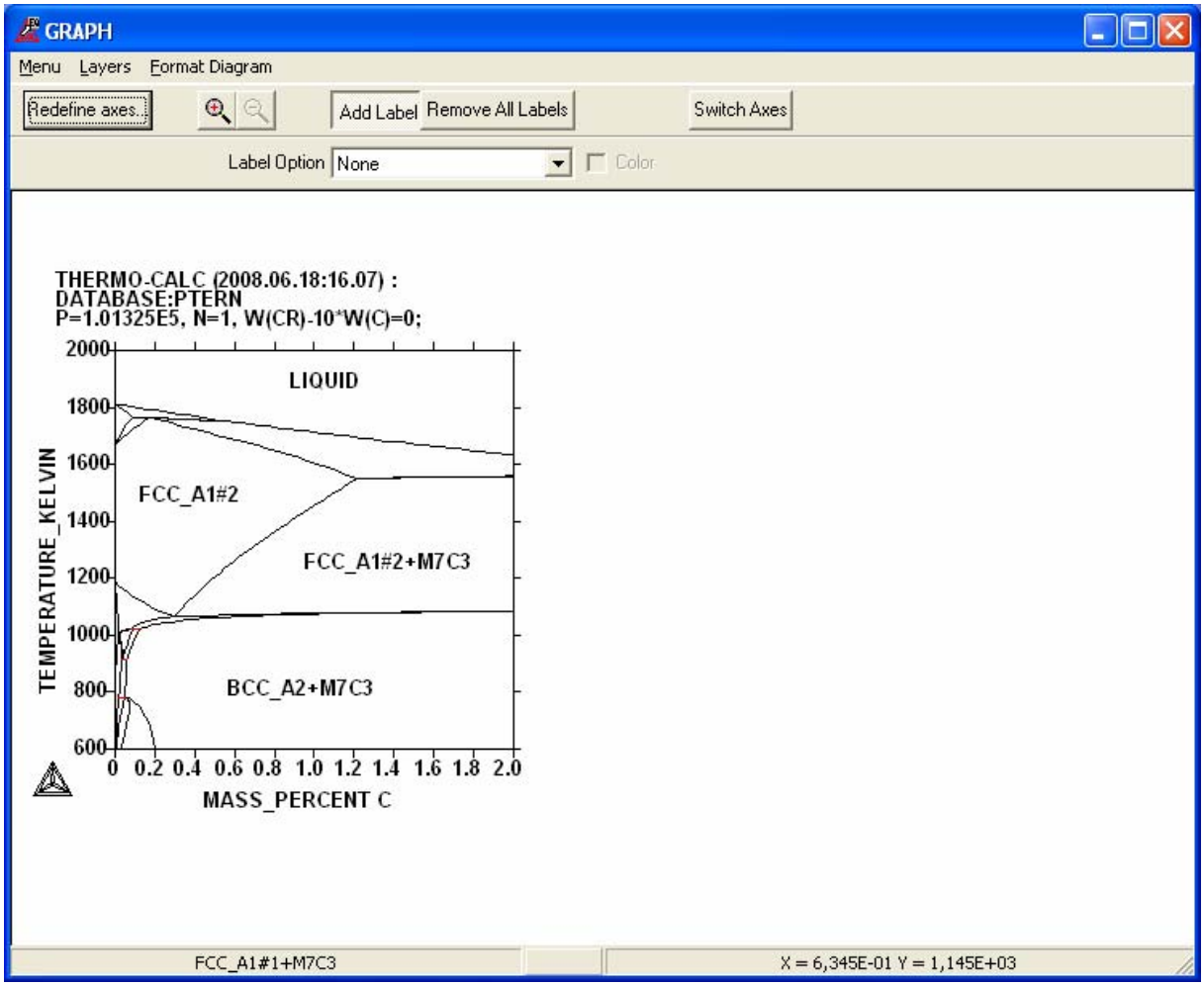
6. Click *Next* and the vertical section is plotted. One can label phase regions by first clicking *Add Label* and clicking in the phase regions one wants to label. The following is a labeled diagram.



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



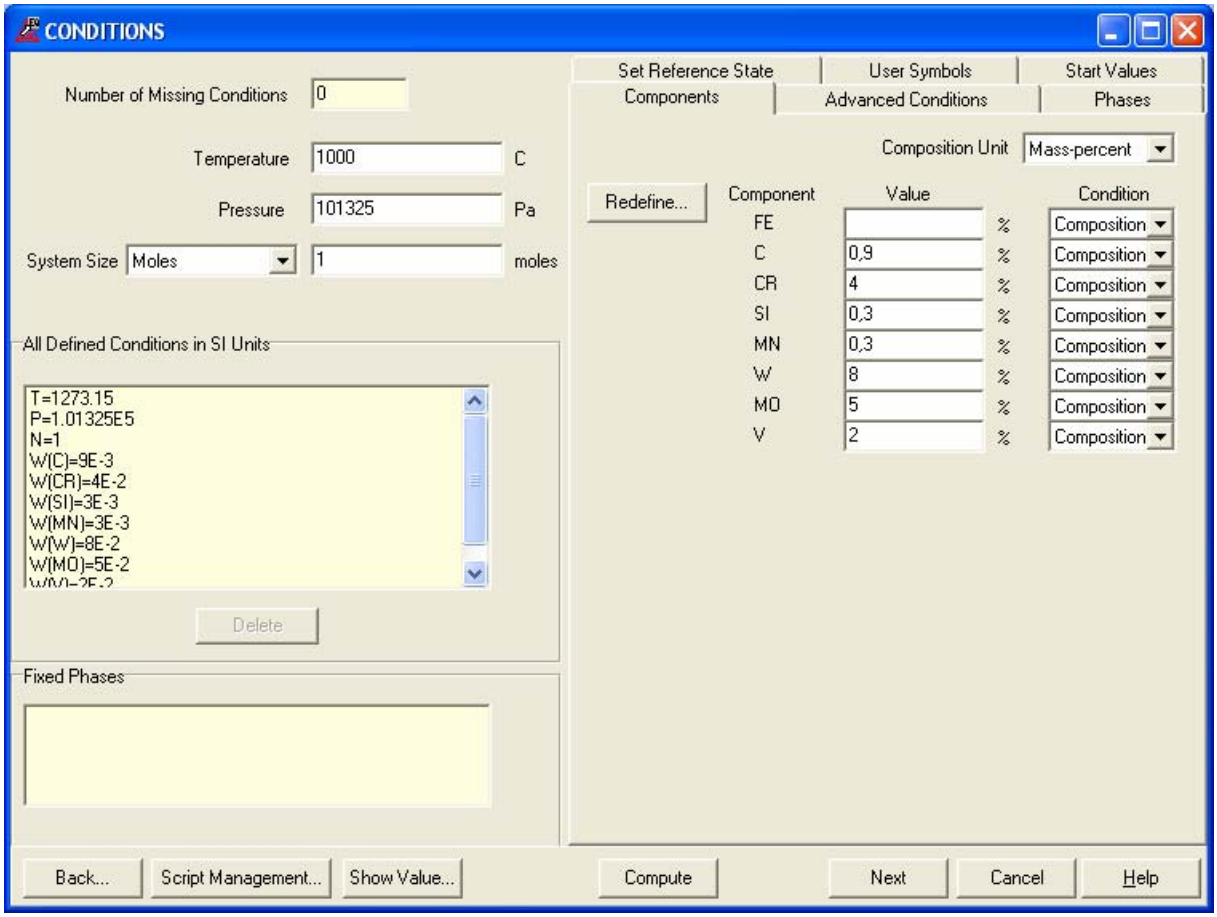
8. Click *Next* and the vertical section is plotted. The following is a labeled diagram.



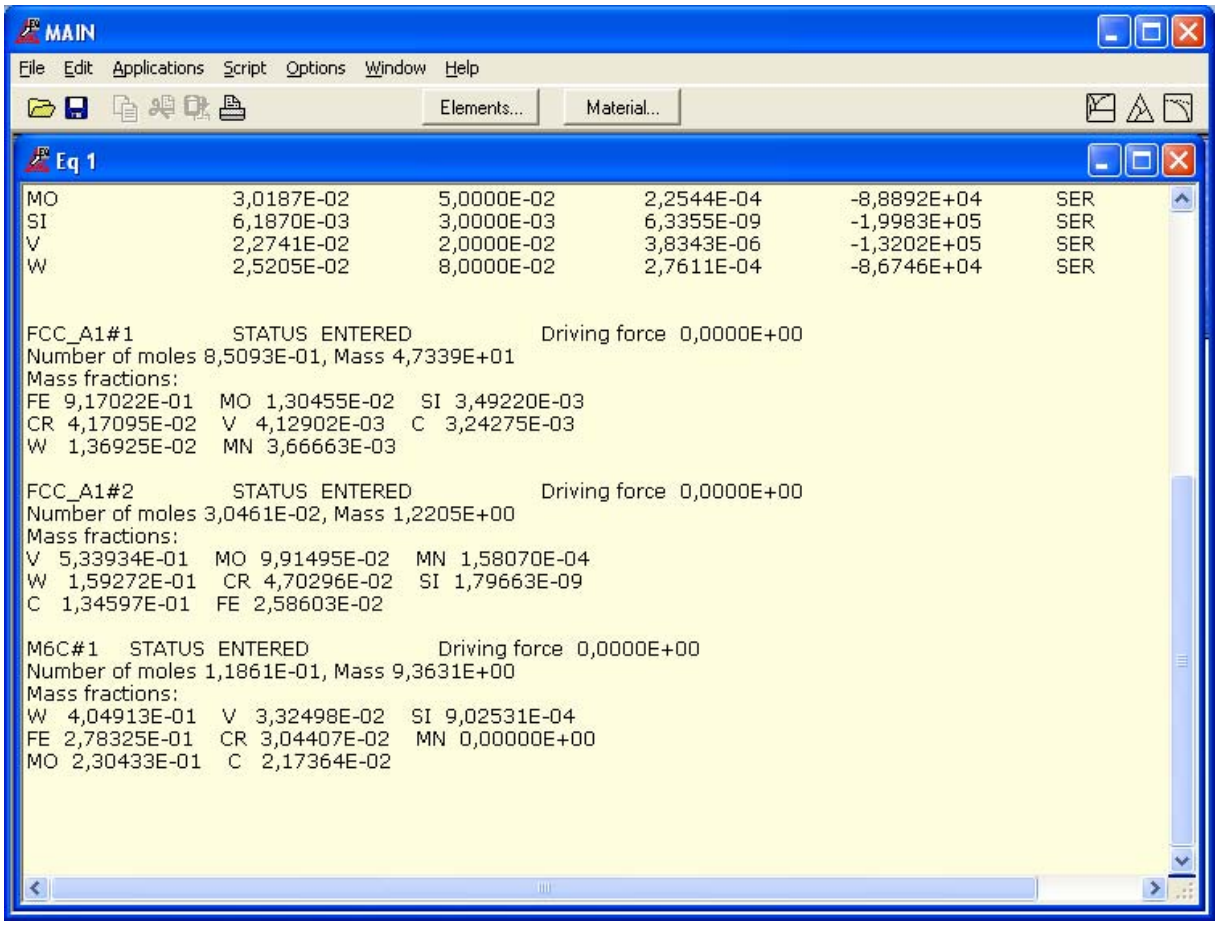
7 Calculation of Property Diagram of a High Speed Steel

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*.

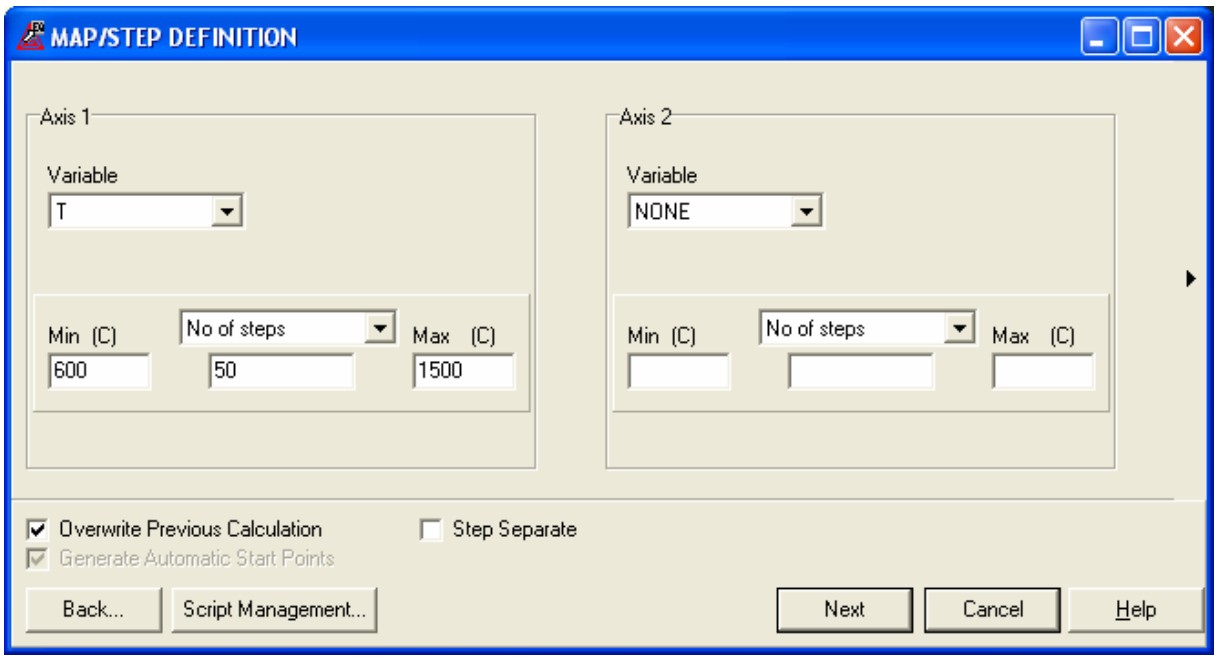
2. Define a single equilibrium in the CONDITIONS window. Put the temperature to *1000* ºC (the default settings for the temperature unit can be changed under the *Options* menu in the MAIN window), and the compositions to *0.9* % C, *4* % Cr, *0.3* % Mn, *5* % Mo, *0.3* % Si, *2* % V and *8* % W (mass %). Fe is the balance, leave the box empty. Now click *Next*.



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.

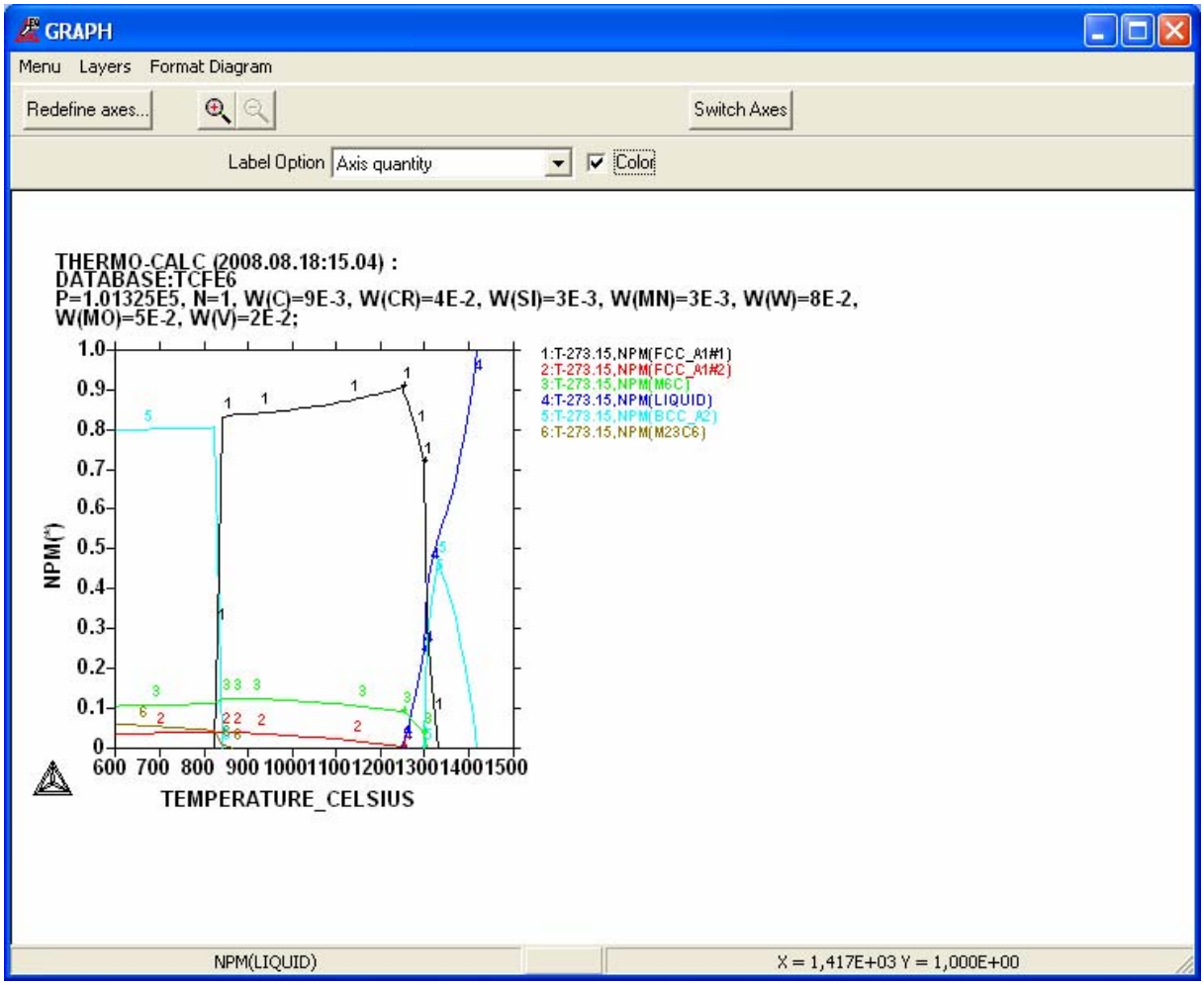


4. The most common property diagram calculation is obtained by stepping in temperature for a given composition. Various temperature dependent quantities can then be used on the Y-axis in the DIAGRAM DEFINITION window. Change axis 1 to *T* and axis 2 to *NONE*. The limits for the temperature axis can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



5. When the step calculation is finished, the DIAGRAM DEFINITION window appears with two axes already defined, let's use these. Press *Next*.

6. 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 ºC, 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 ºC.



7. 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.

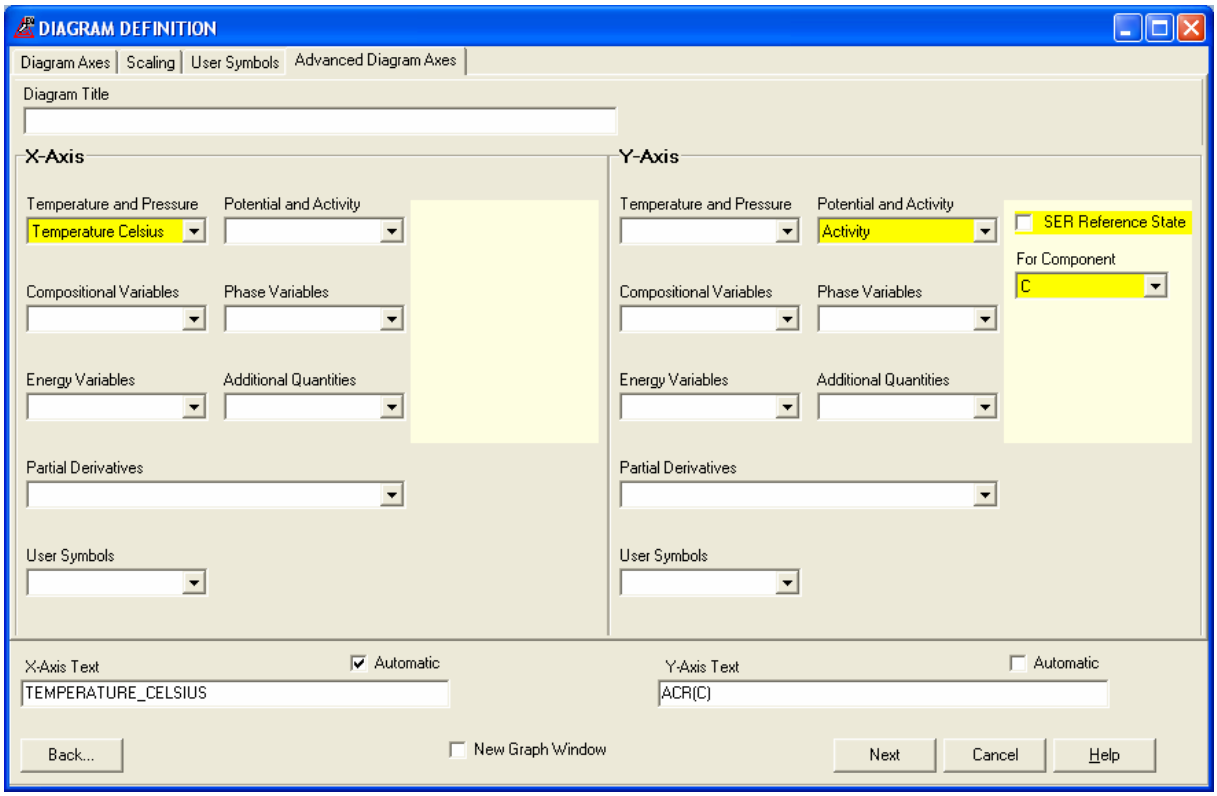
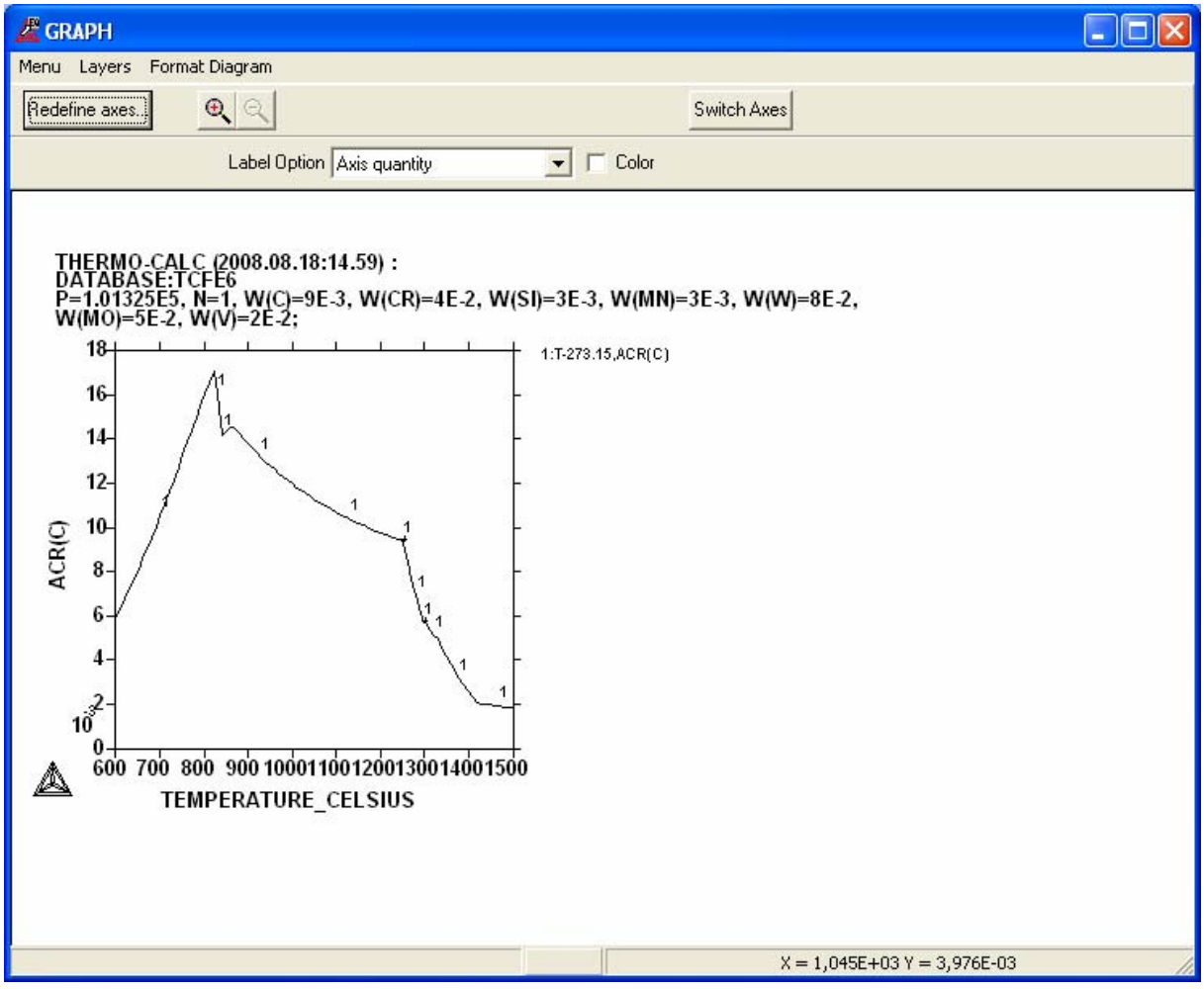
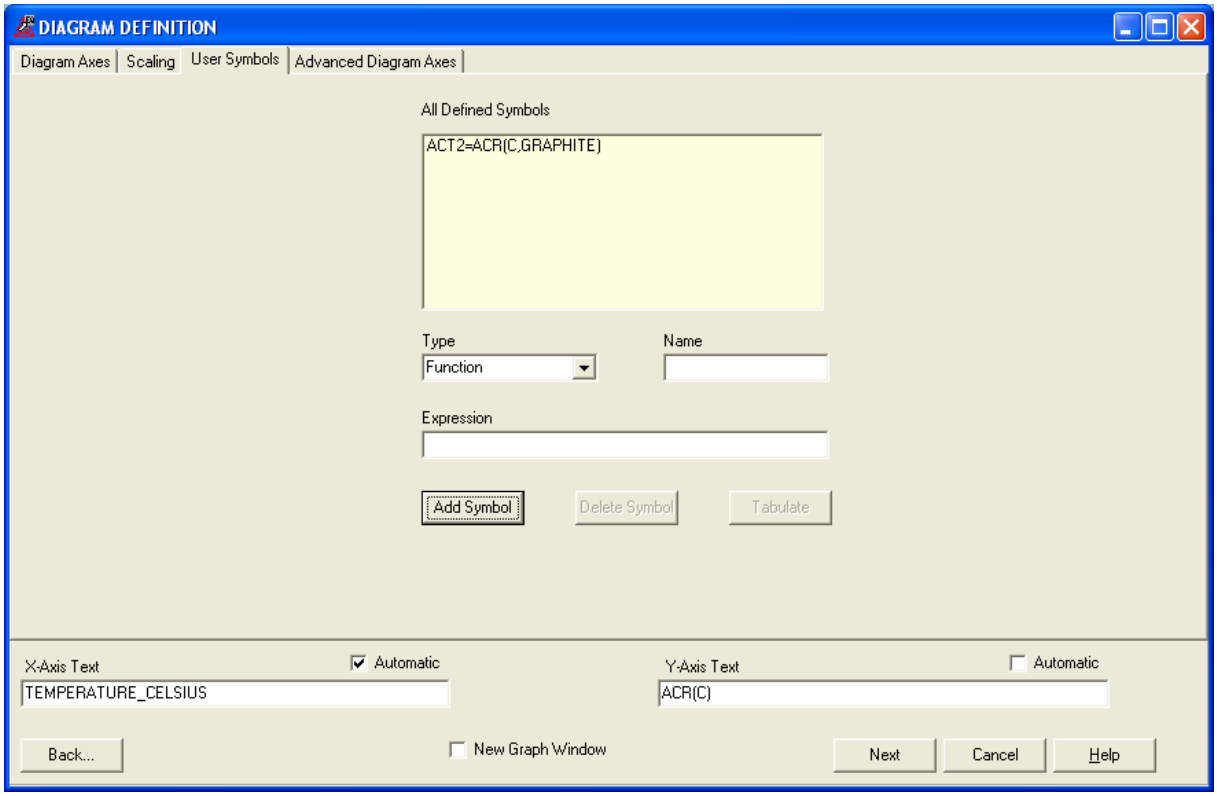
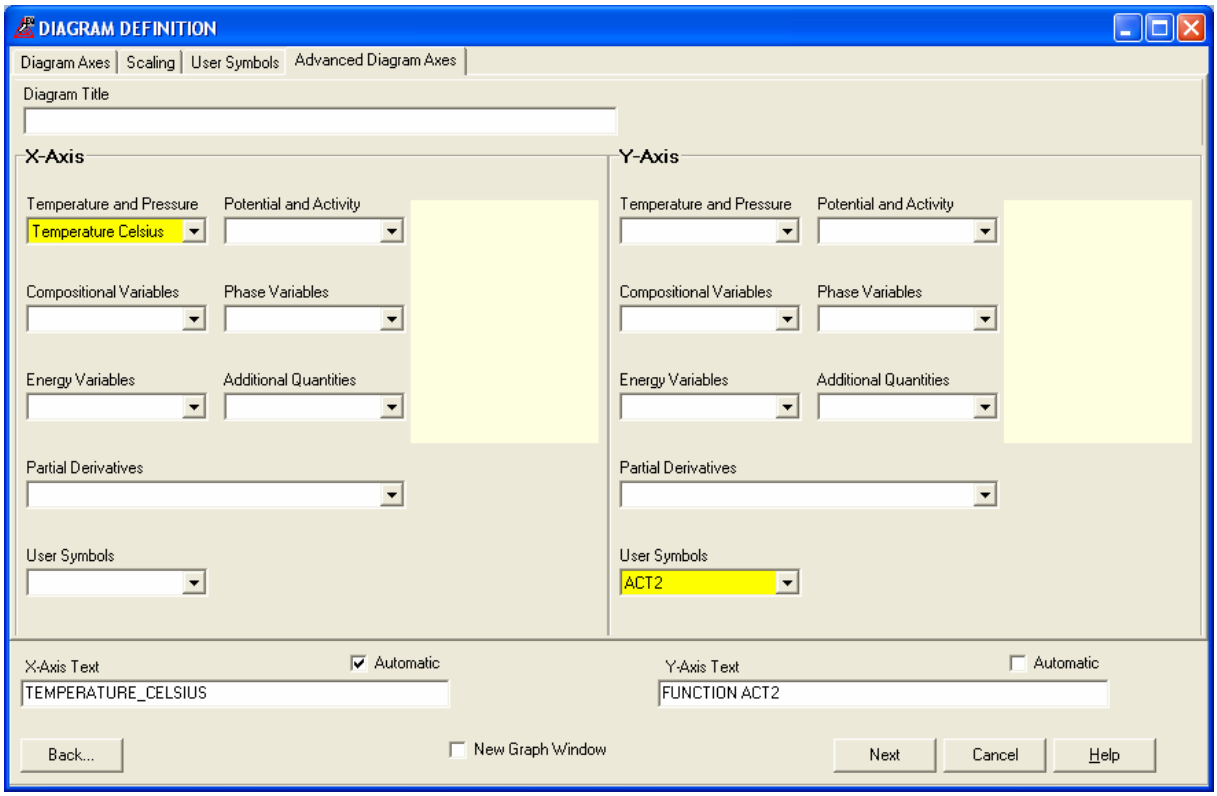


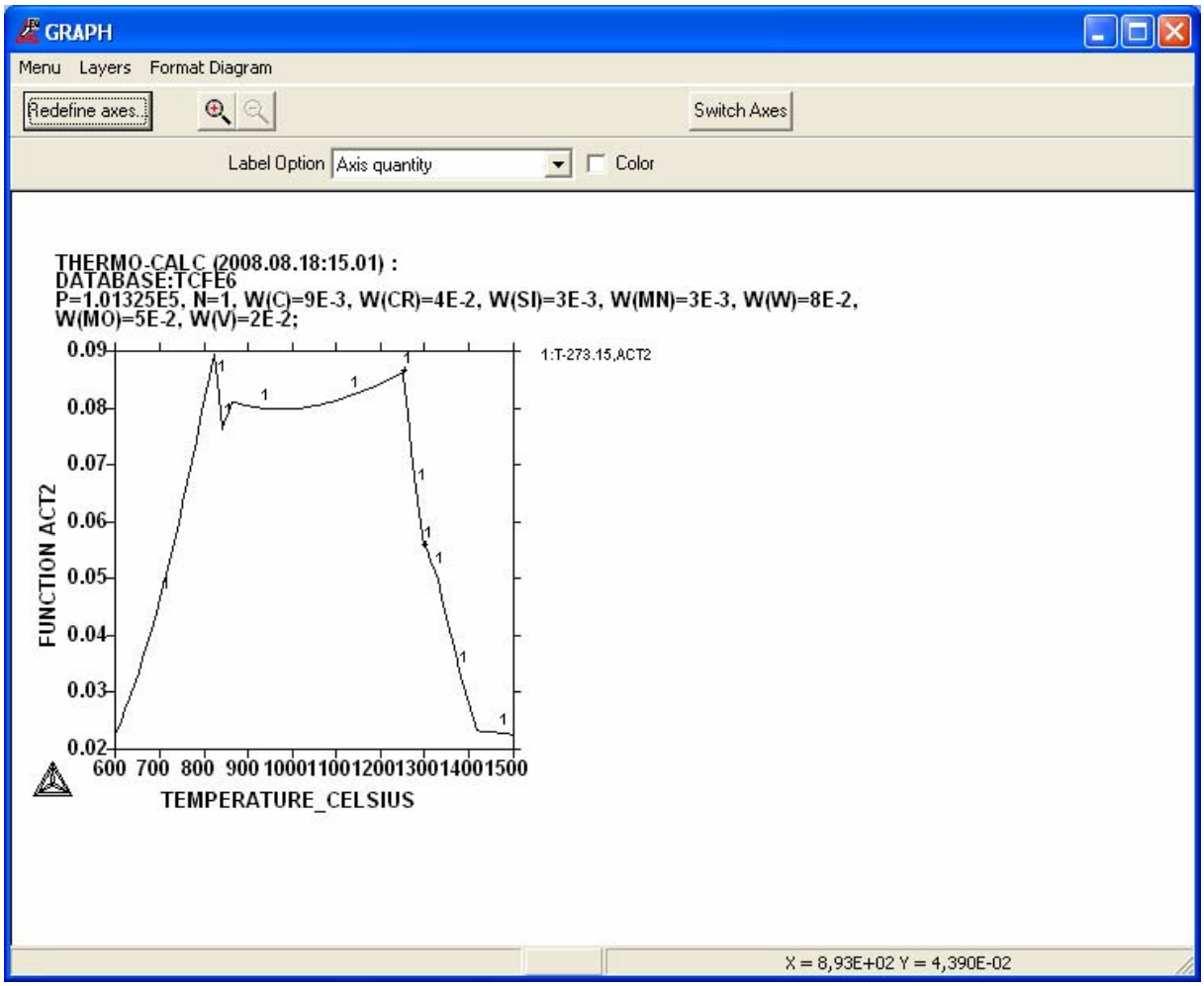
DIAGRAM DEFINITION
Diagram Axes
Scaling
User Symbols
Advanced Diagram Axes
Diagram Title
X-Axis
Temperature and Pressure
Temperature Celsius
Potential and Activity
Compositional Variables
Phase Variables
Energy Variables
Additional Quantities
Partial Derivatives
User Symbols
Y-Axis
Temperature and Pressure
Potential and Activity
Activity
SER Reference State
For Component
C
Compositional Variables
Phase Variables
Energy Variables
Additional Quantities
Partial Derivatives
User Symbols
X-Axis Text
Automatic
TEMPERATURE_CELSIUS
Y-Axis Text
Automatic
ACR(C)
Back...
New Graph Window
Next
Cancel
Help


GRAPH
Menu
Layers
Format Diagram
Redefine axes...
Switch Axes
Label Option
Axis quantity
Color
THERMO-CALC (2008.08.18:14.59) :
DATABASE:TCFE6
P=1.01325E5, N=1, W(C)=9E-3, W(CR)=4E-2, W(SI)=3E-3, W(MN)=3E-3, W(W)=8E-2,
W(MO)=5E-2, W(V)=2E-2;
1:T-273.15,ACR(C)
ACR(C)
TEMPERATURE_CELSIUS
X = 1,045E+03 Y = 3,976E-03

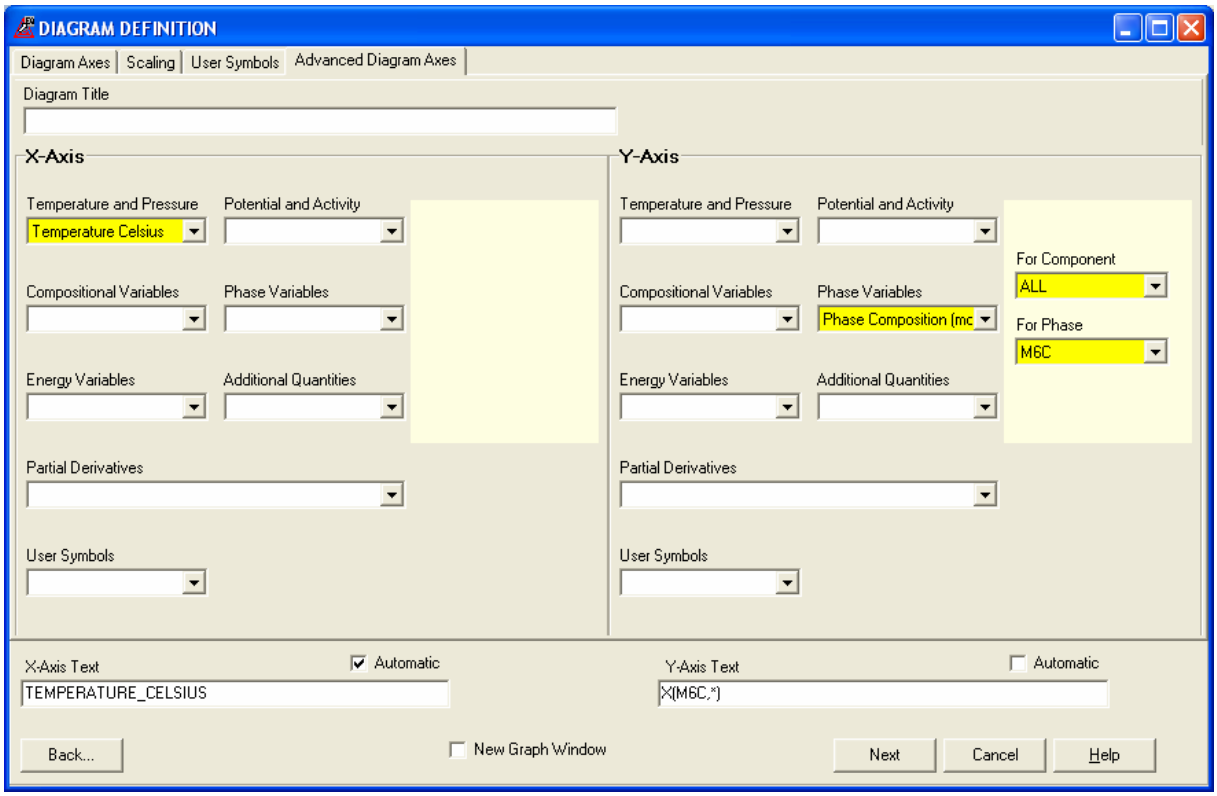
8. The magnitude of the carbon activity may seem strange in the last plot. This is because the default reference state for carbon is at room temperature in this database. Enter a function to refer the C activity to graphite at the temperature of the calculation. Click *Redefine* and open the *User Symbols* 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.



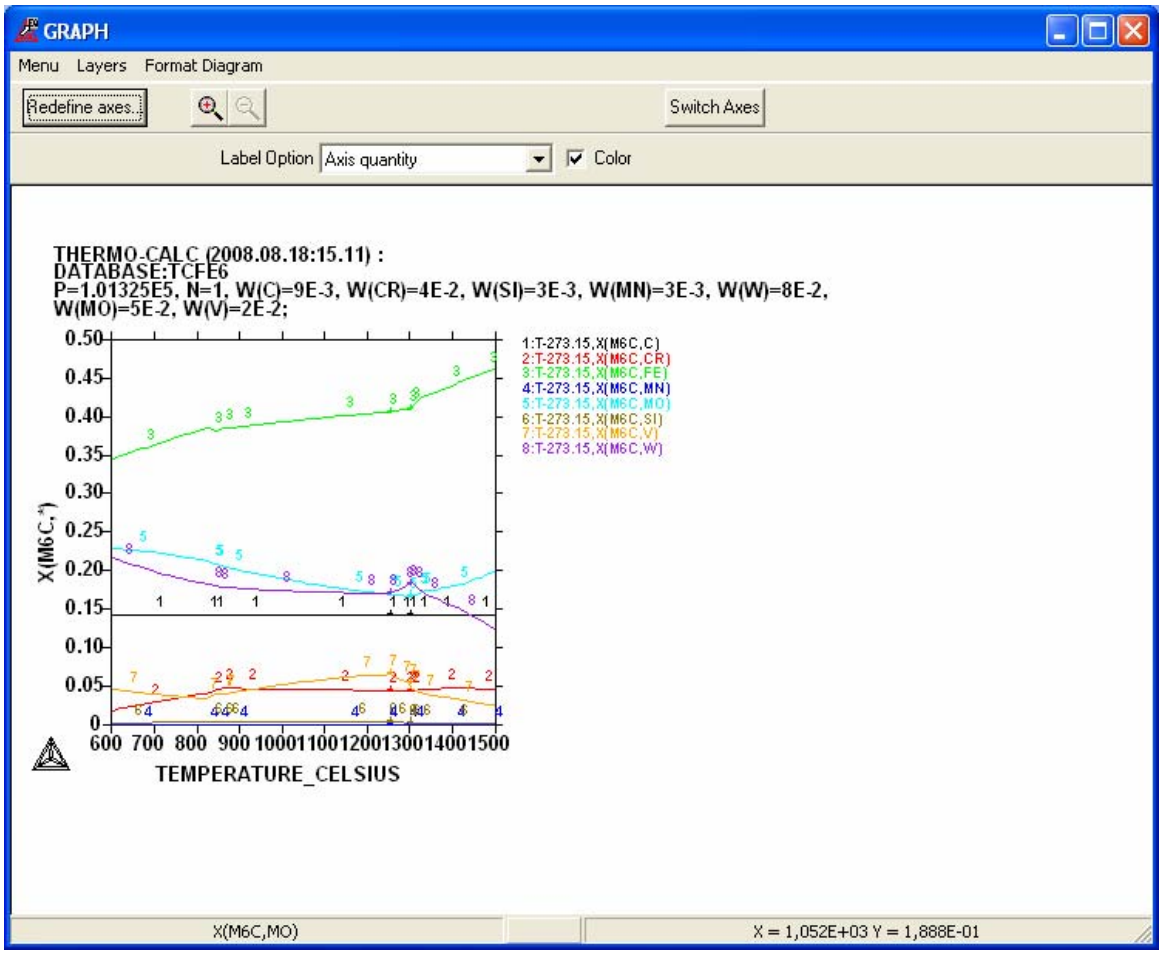




9. Click *Redefine* to plot yet another property diagram, this time the composition of the M6C phase. Open the *Advaced Diagram Axes* tab and select *Phase Composition (moles)* for all components in the M6C phase as the Y-axis variable. Click *Next* to plot. In the diagram below, note that the M6C phase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



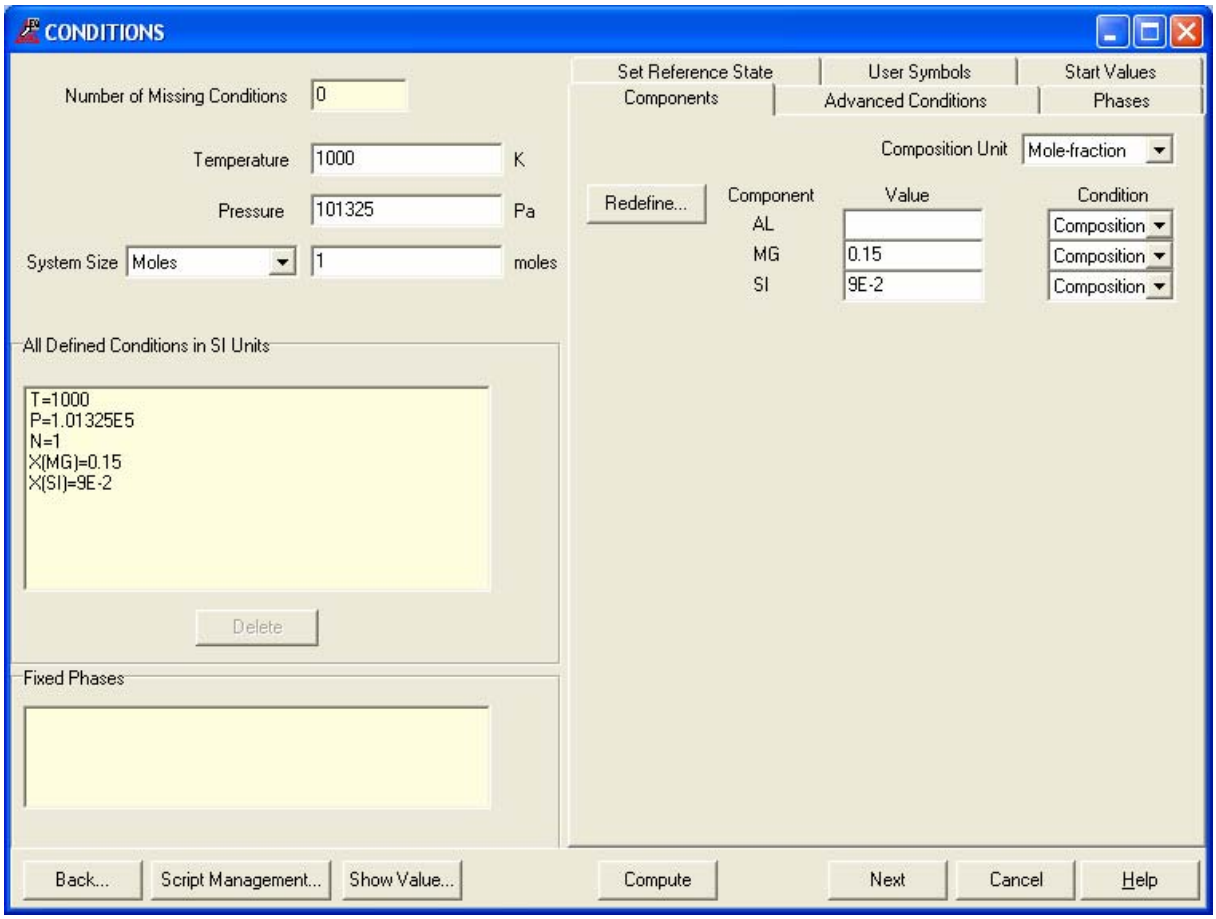
10. Select *Axis quantity* in the *Label Option* menu and check the color box.



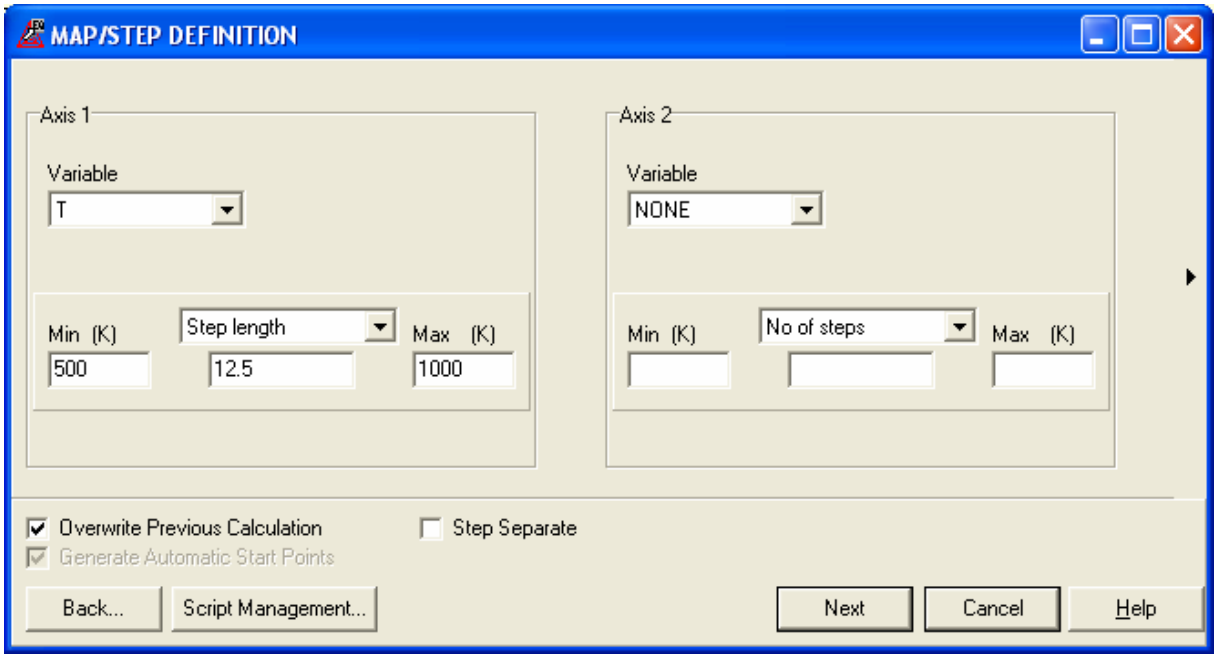
8 Calculate Heat and Heat Capacity Variation during Solidification of an Al-15%Mg-9%Si Alloy

1. Click the *Elements* button in the MAIN window. Select database *PTERN* and elements *Al*, *Mg* and *Si* from the periodic table.

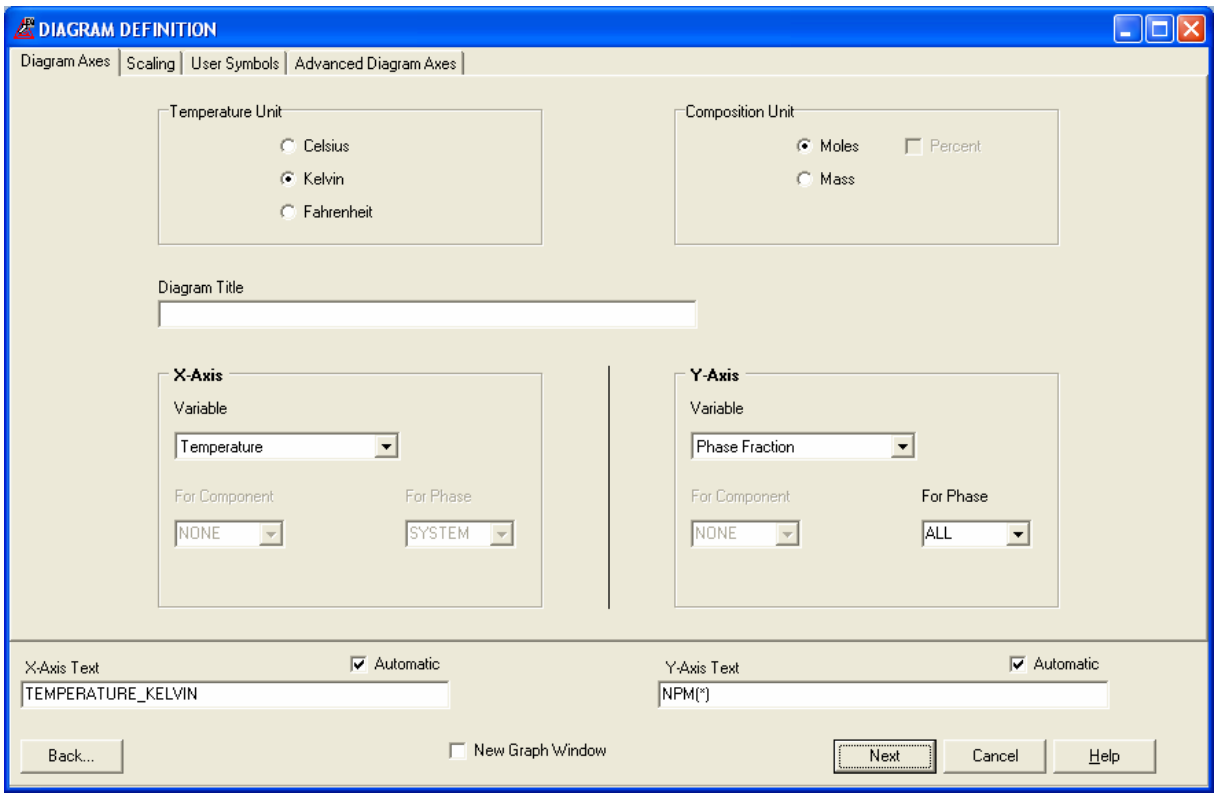
2. Click *Next* to come to the CONDITIONS window. Enter compositions in mass-fraction; 0.15 Mg and 0.09 Si, and the temperature 1000 K.

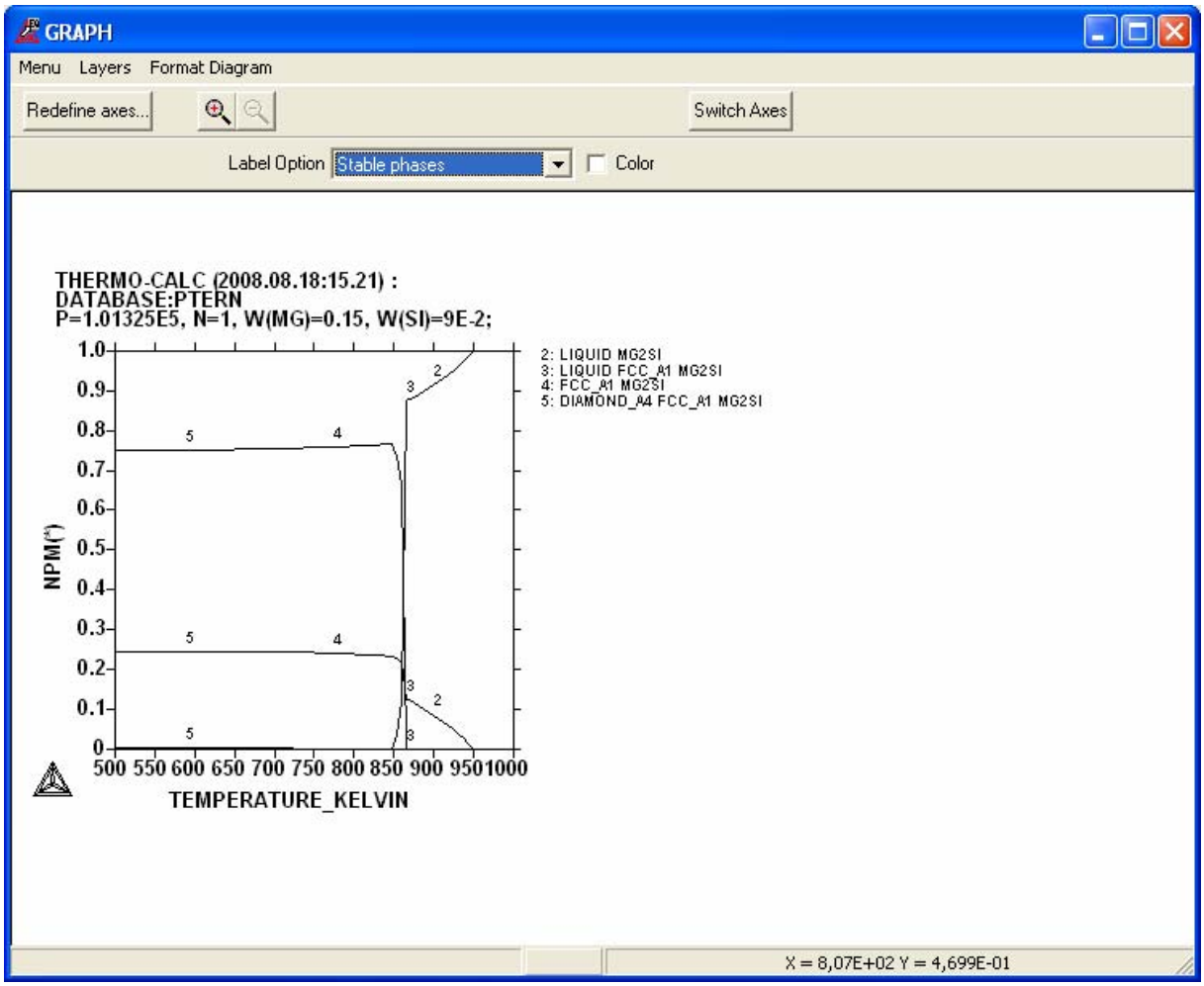


3. Click next to open the MAP/STEP DEFINITION window. Set *T* as axis variable and step between *500 K* and *1000 K* with step length *12.5*. Click *Next*.



4. 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.





5. 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.

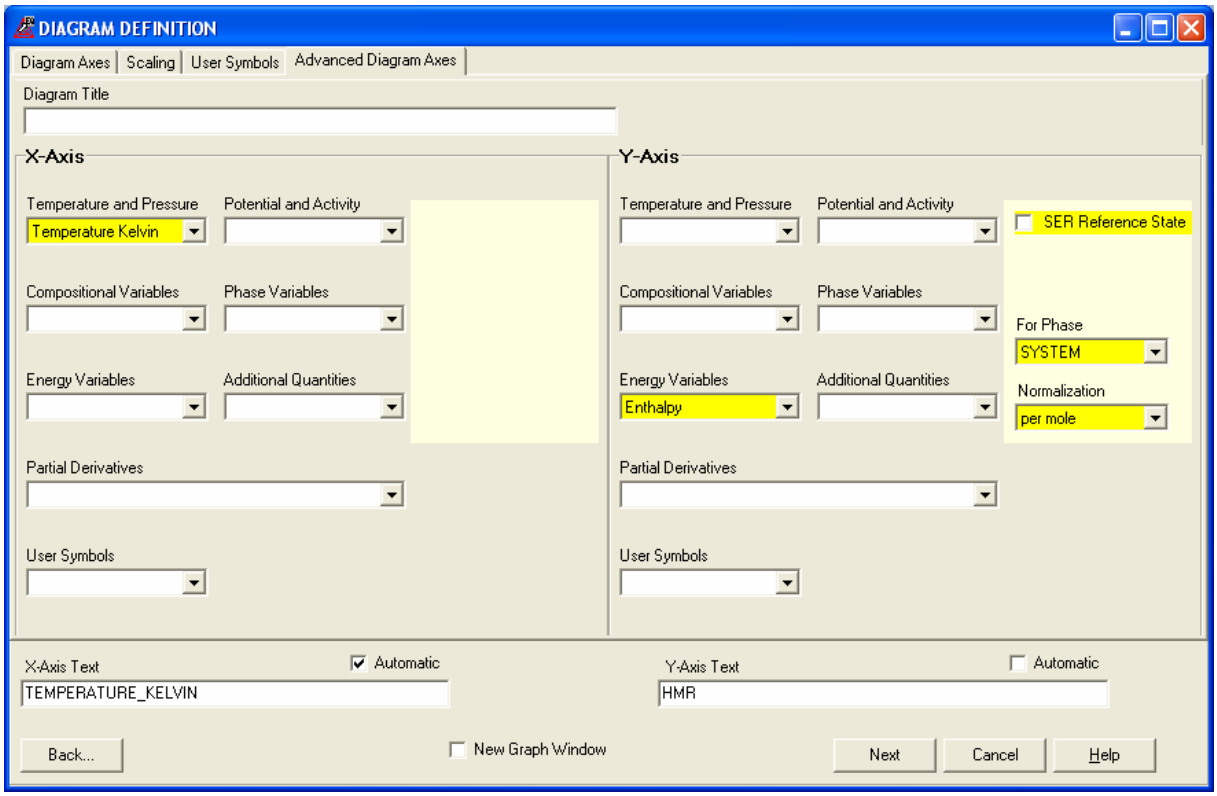
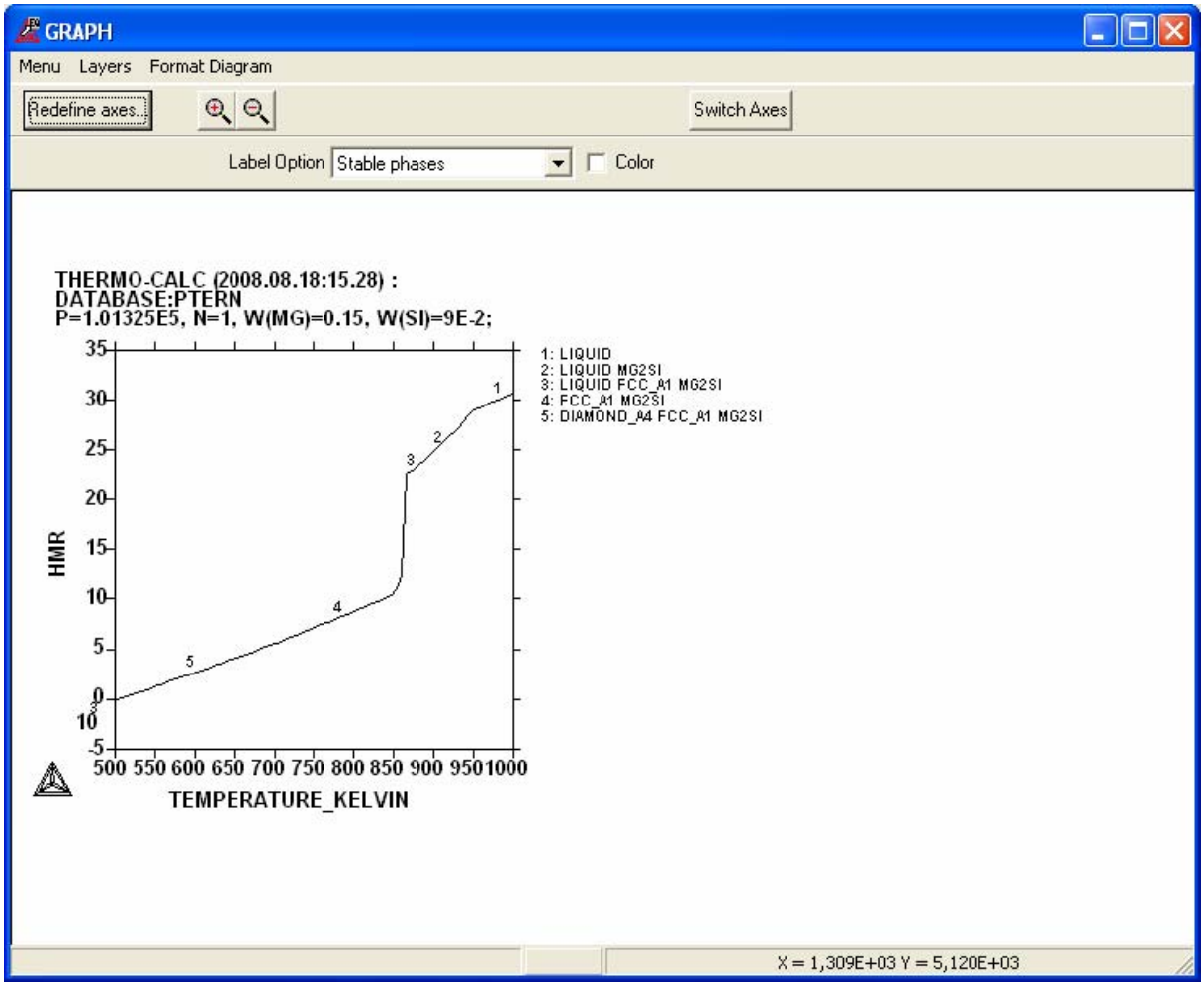
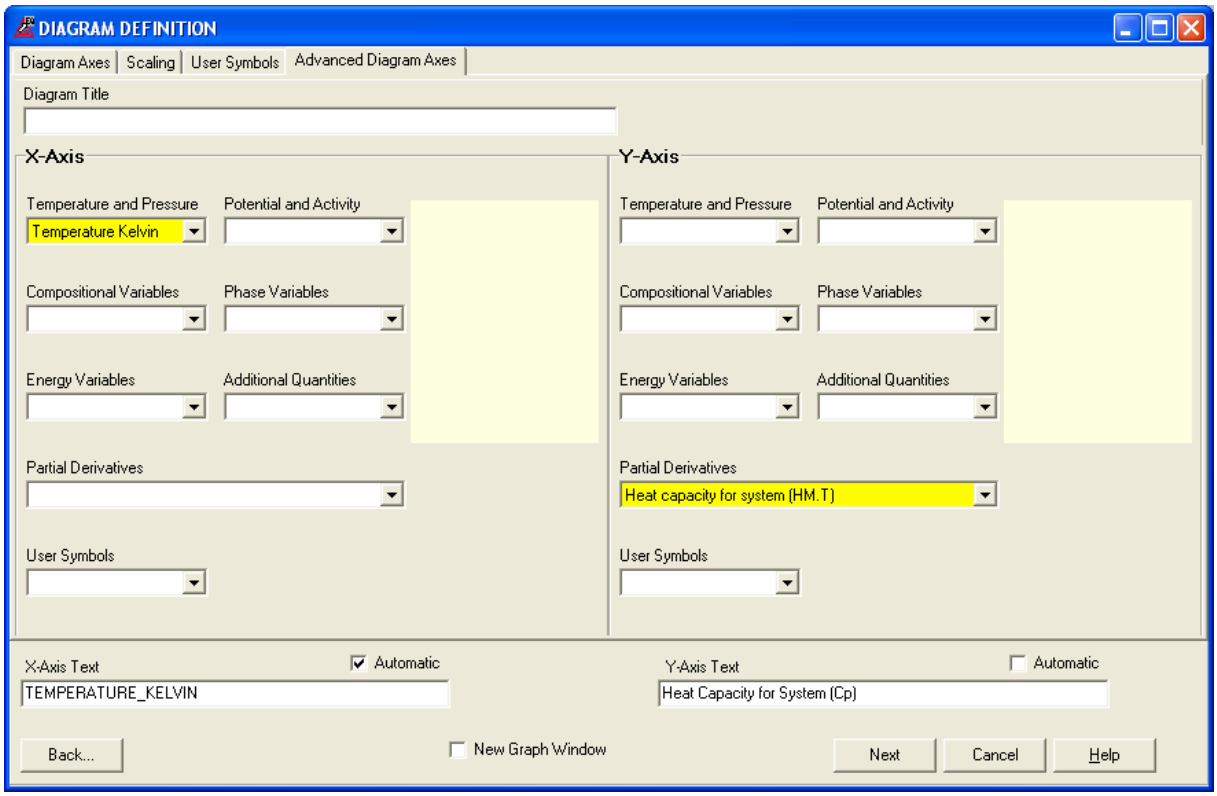
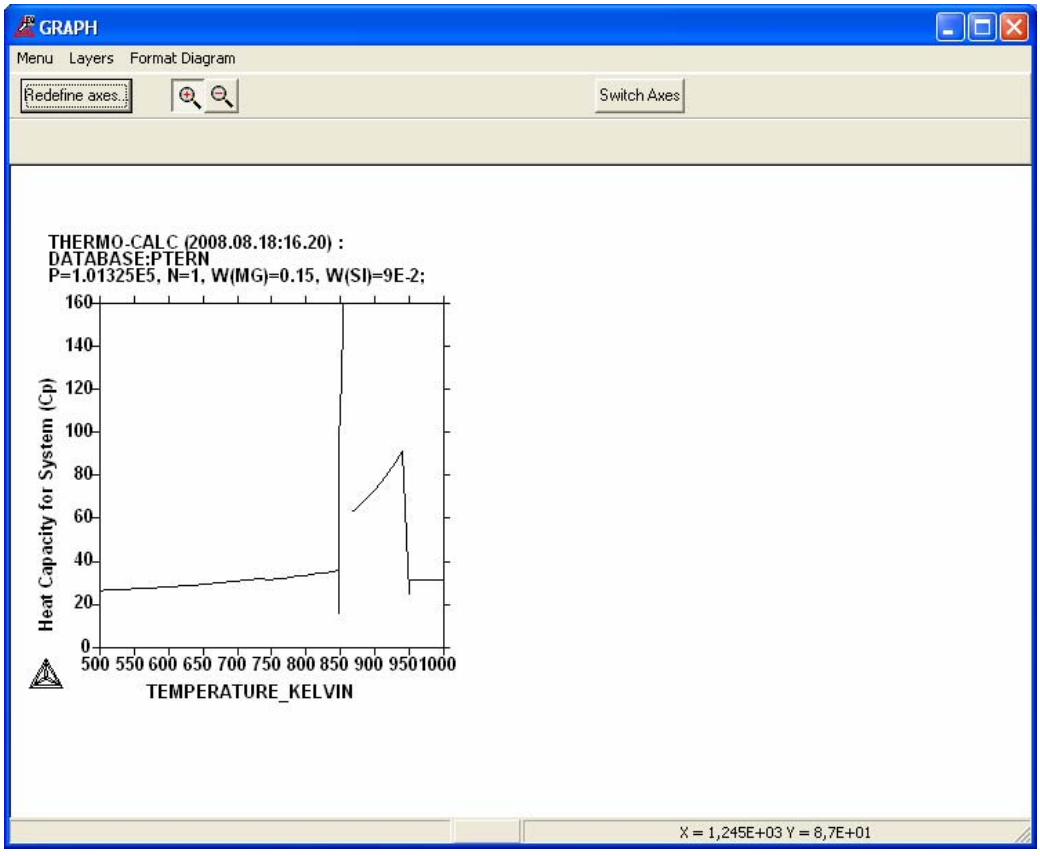


DIAGRAM DEFINITION
Diagram Axes
Scaling
User Symbols
Advanced Diagram Axes
Diagram Title
X-Axis
Temperature and Pressure
Temperature Kelvin
Potential and Activity
Compositional Variables
Phase Variables
Energy Variables
Additional Quantities
Partial Derivatives
User Symbols
Y-Axis
Temperature and Pressure
Potential and Activity
SER Reference State
Compositional Variables
Phase Variables
For Phase
SYSTEM
Energy Variables
Enthalpy
Additional Quantities
Normalization
per mole
Partial Derivatives
User Symbols
X-Axis Text
Automatic
TEMPERATURE_KELVIN
Y-Axis Text
Automatic
HMR
Back...
New Graph Window
Next
Cancel
Help


GRAPH
Menu
Layers
Format Diagram
Redefine axes...
Switch Axes
Label Option
Stable phases
Color
THERMO-CALC (2008.08.18:15.28) :
DATABASE:PTERN
P=1.01325E5, N=1, W(MG)=0.15, W(SI)=9E-2;
1: LIQUID
2: LIQUID MG2SI
3: LIQUID FCC_A1 MG2SI
4: FCC_A1 MG2SI
5: DIAMOND_A4 FCC_A1 MG2SI
HMR
35
30
25
20
15
10
5
0
-5
10^3
500 550 600 650 700 750 800 850 900 950 1000
TEMPERATURE_KELVIN
X = 1,309E+03 Y = 5,120E+03

6. 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.

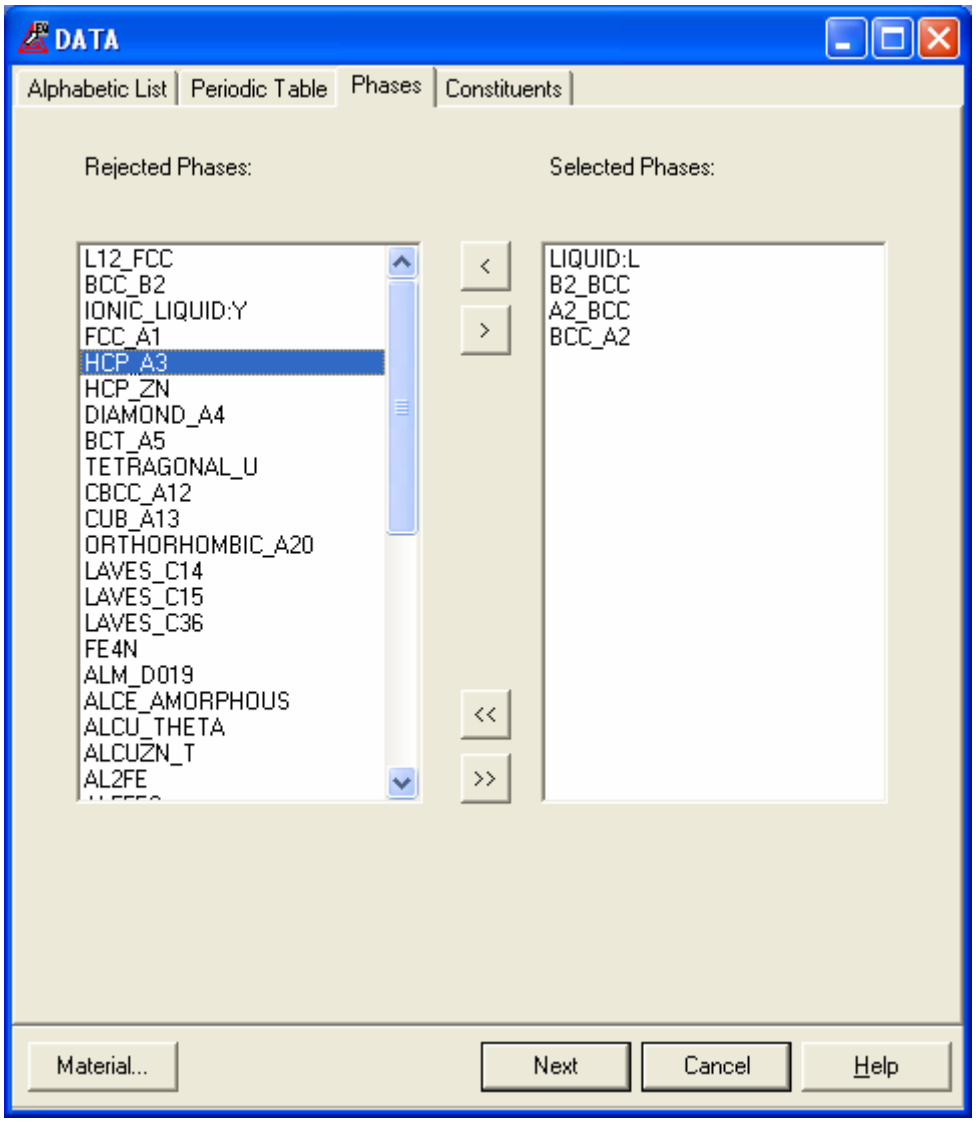




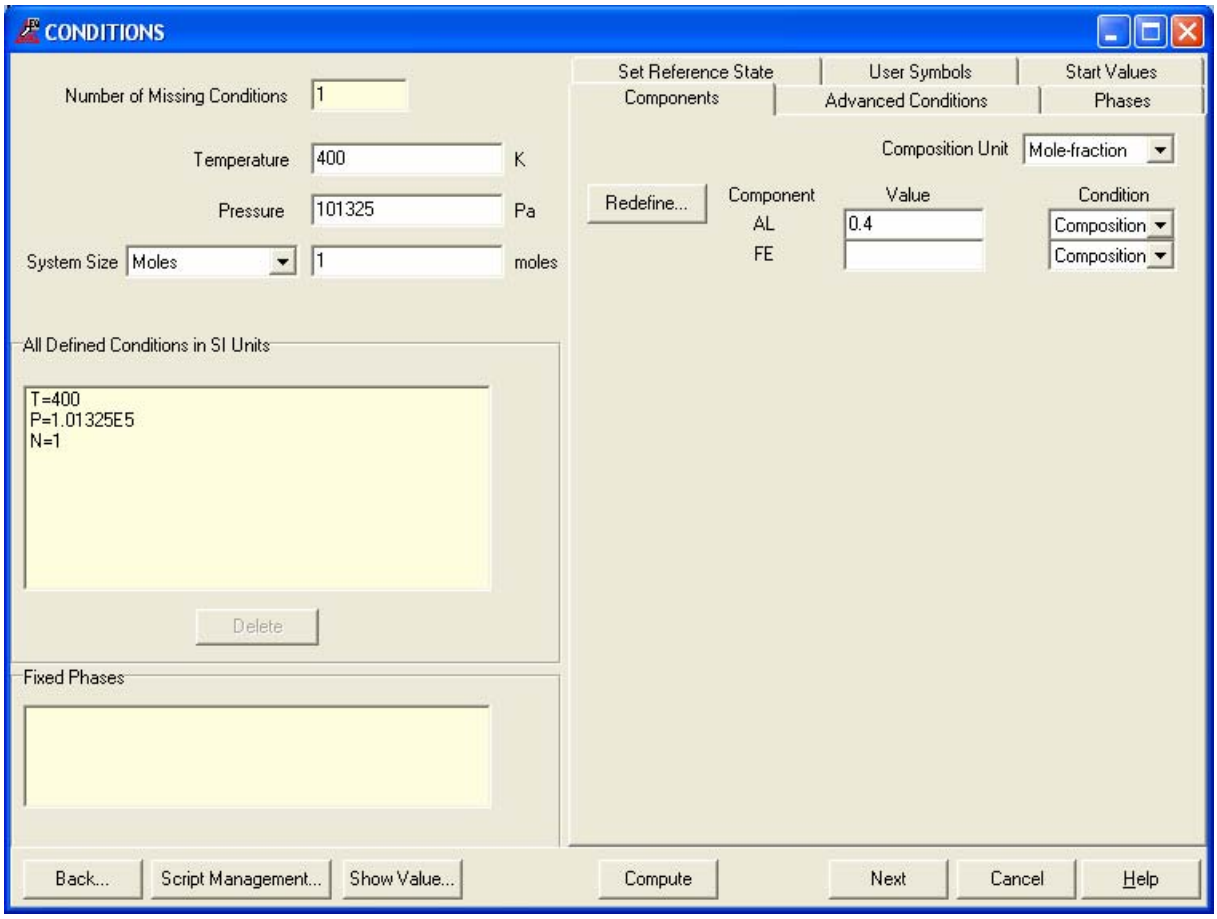
9 Calculate Second Order Transition Line in Al-Fe System

1. Click the *Elements* button in the MAIN window and select database *SSOL4* and elements *Al* and *Fe* from the periodic table.

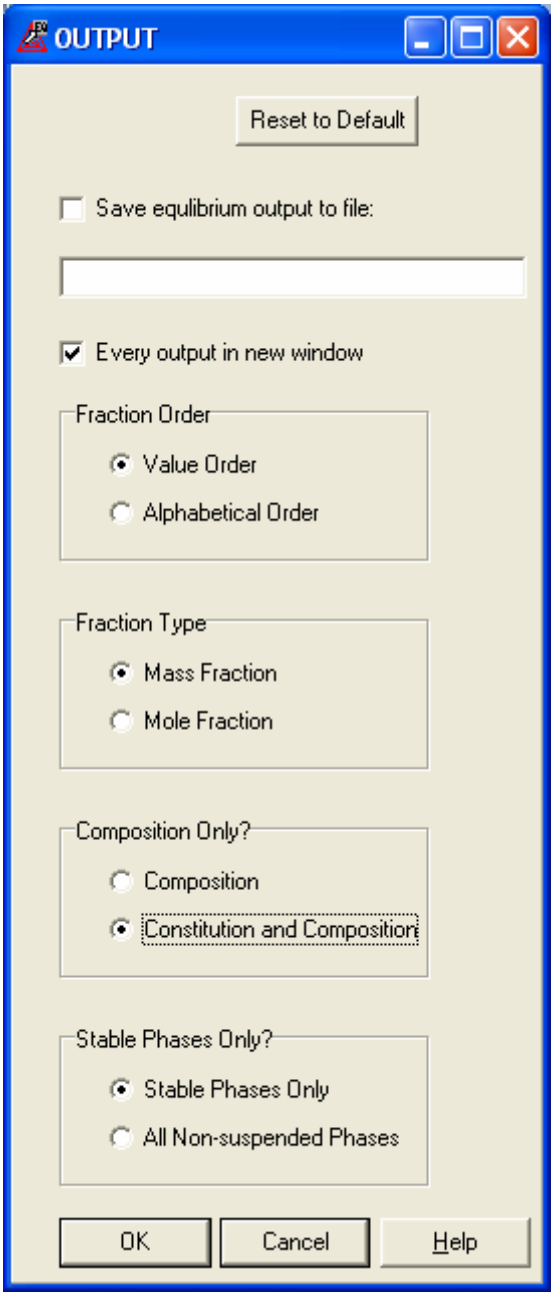
2. Reject all phases and select *LIQUID, B2_BCC, BCC_A2 and A2_BCC (disordered part of the B2_BCC)*.

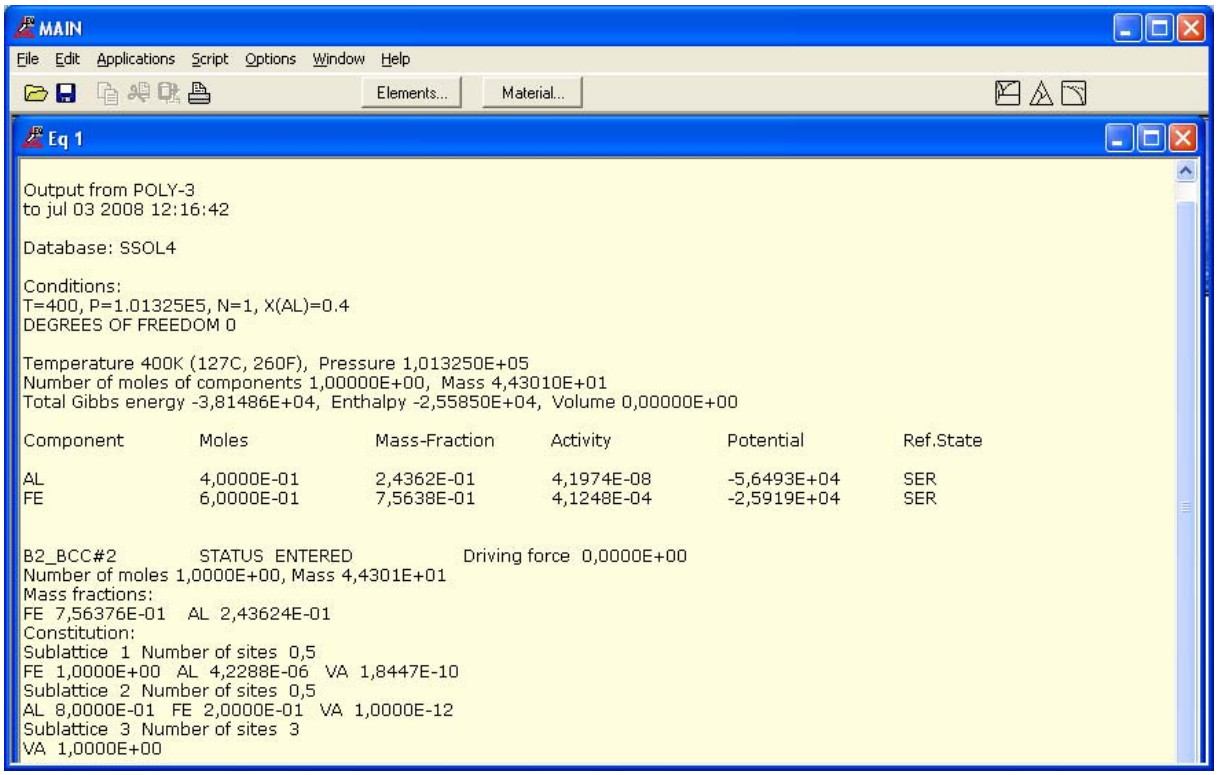


3. Click *Next* to come to the CONDITIONS window. Select the composition unit mole-fraction and set the amount of Al to 0.4, and the temperature to 400 K.



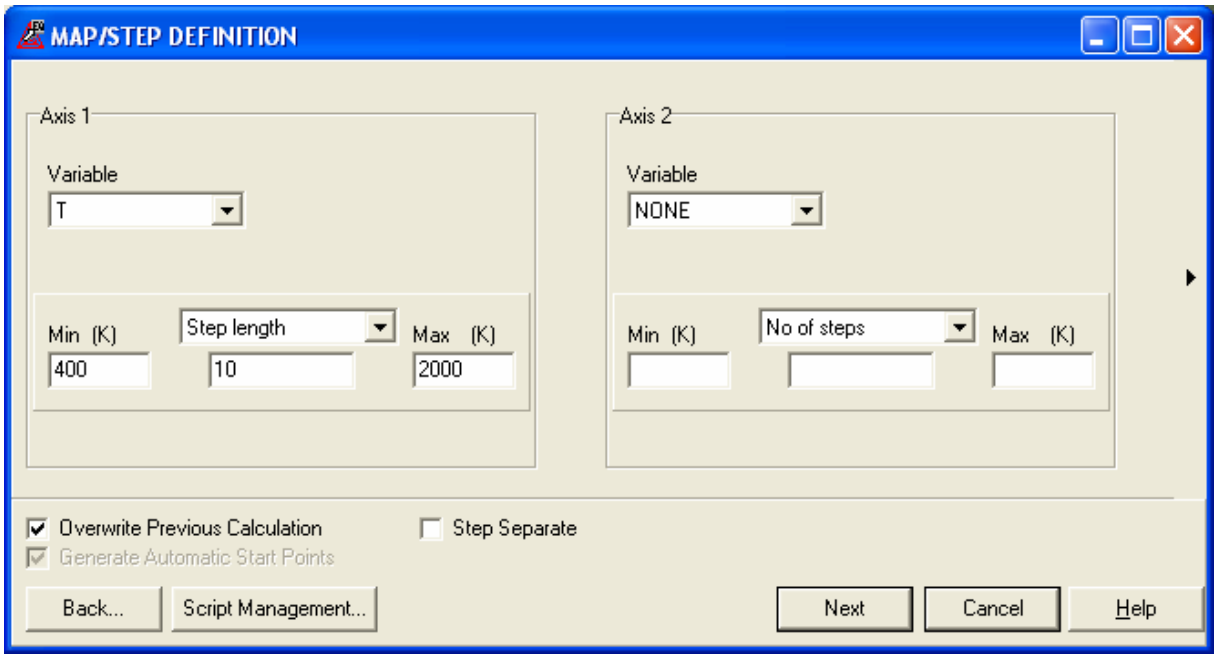
4. To see how Al and Fe distribute on the sublattices click the *Options* in the MAIN window and select *Output.* Select *Constitution and Composition* and click *Ok,* then click *Compute*.


OUTPUT
Reset to Default
Save equlibrium 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
OK
Cancel
Help

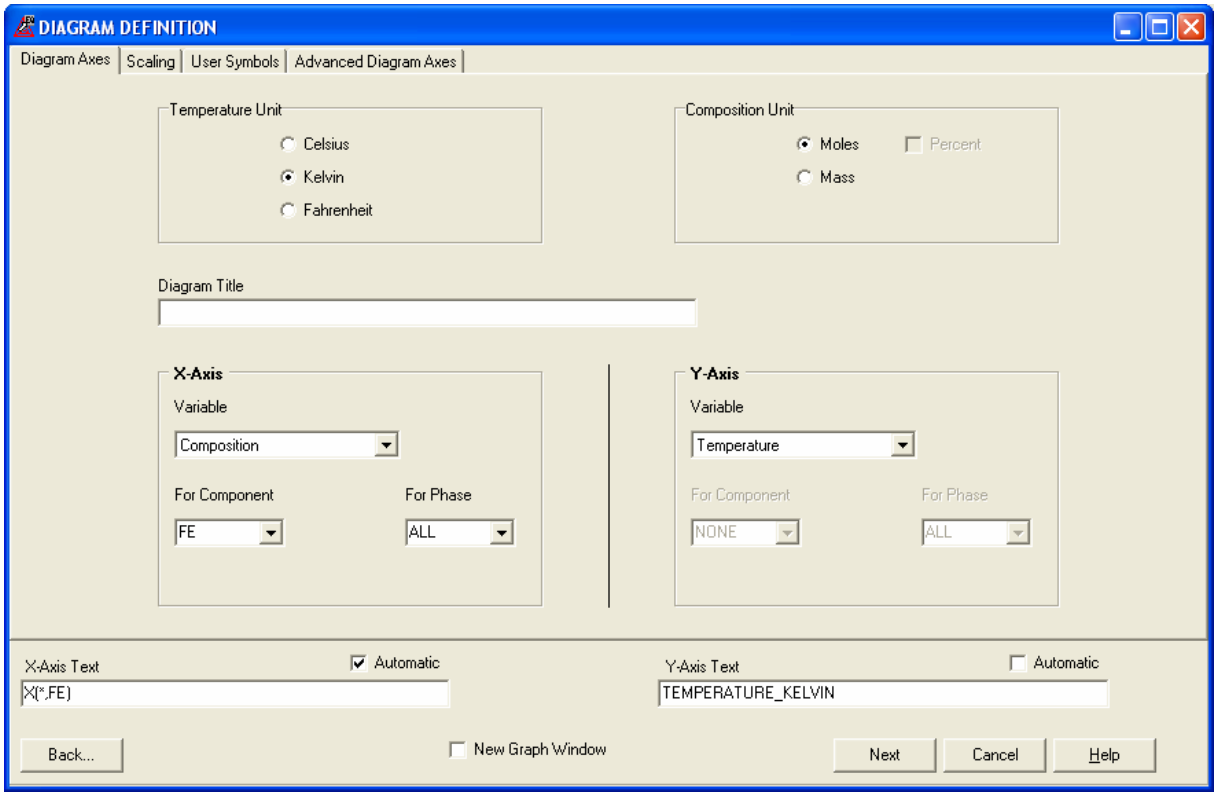


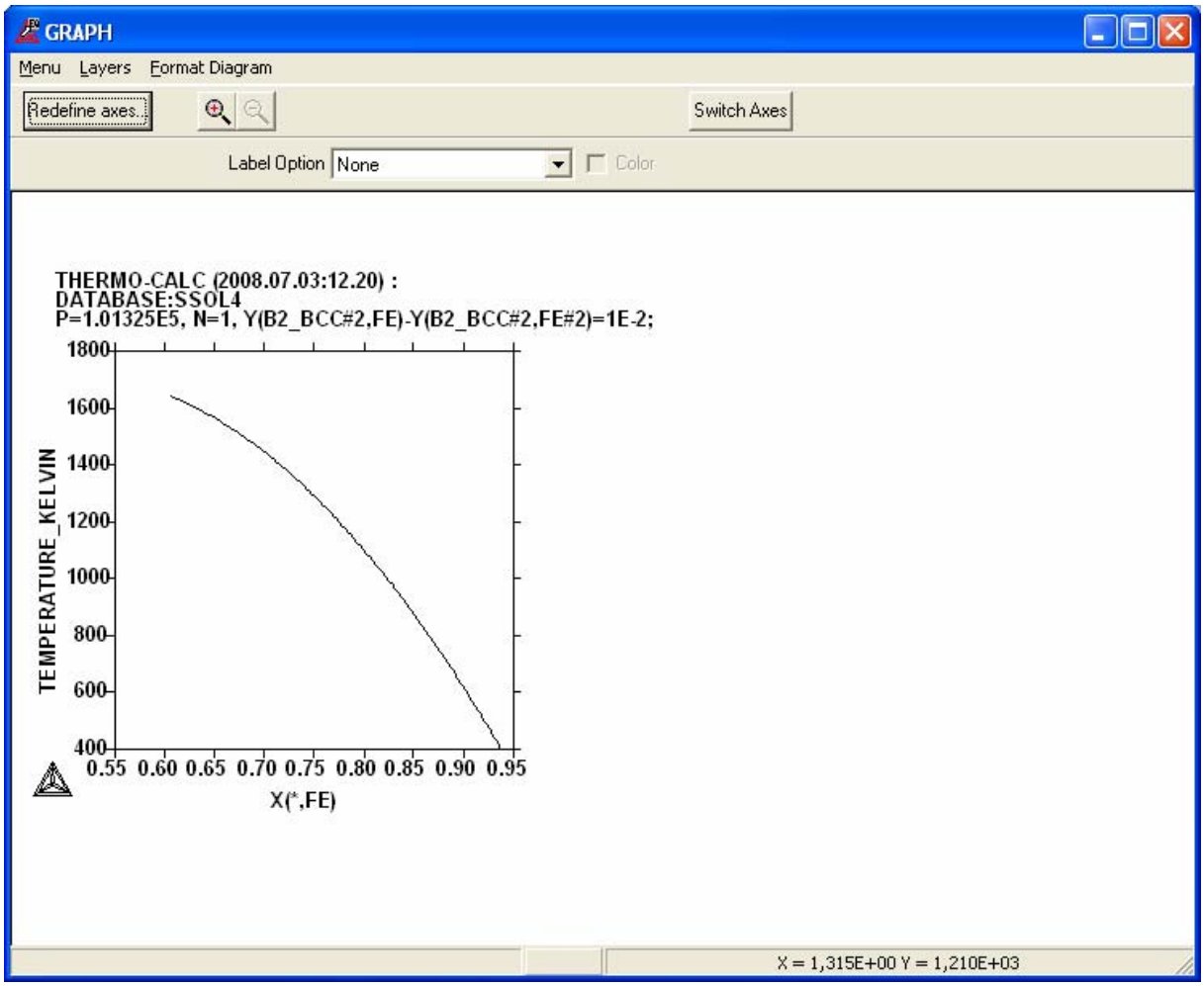
5. Change the condition for the amount of Al to be that of a difference in site-fractions in the two sublattices. Remove the *X(AL)=0.4* condition and enter *Y(B2_BCC#2,FE#1)-Y(B2_BCC#2,FE#2)=1E-2* under the *Advanced Conditions* tab in the CONDITIONS window.

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*.

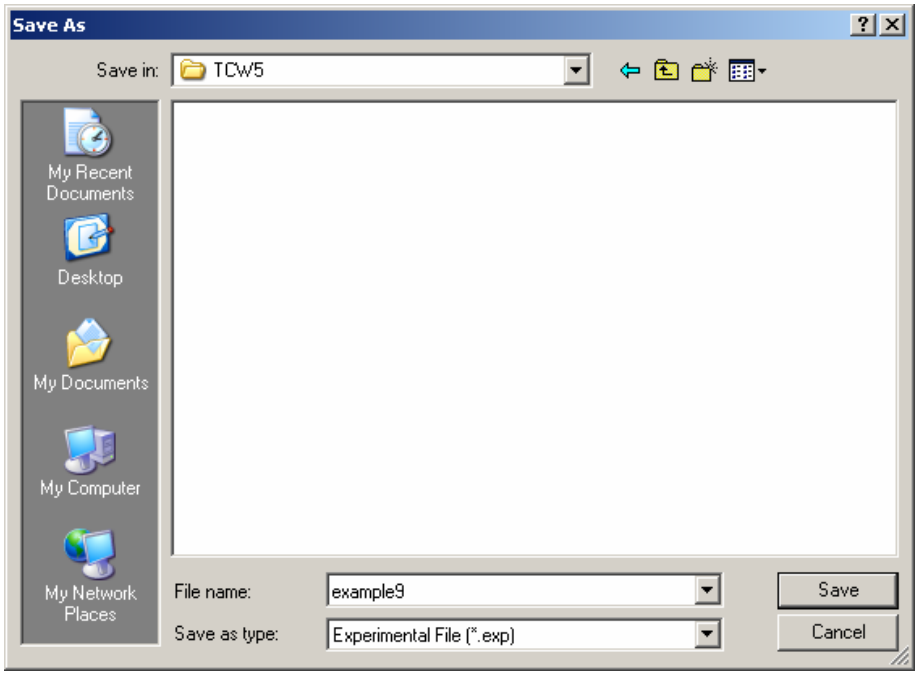


7. Select *Mole-Fraction* of *Fe* in *All* phases and *Temperature* as diagram axes. Click *Next* to plot.

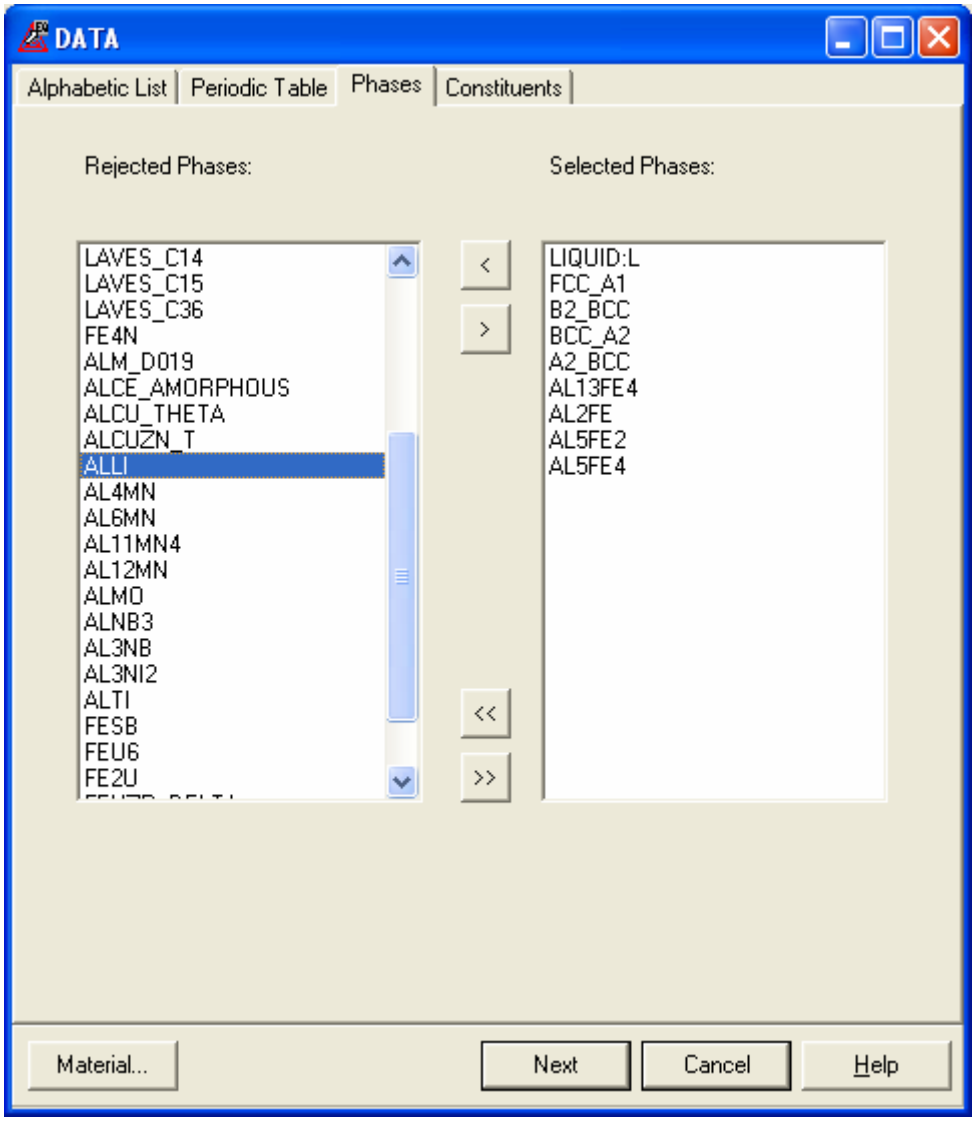




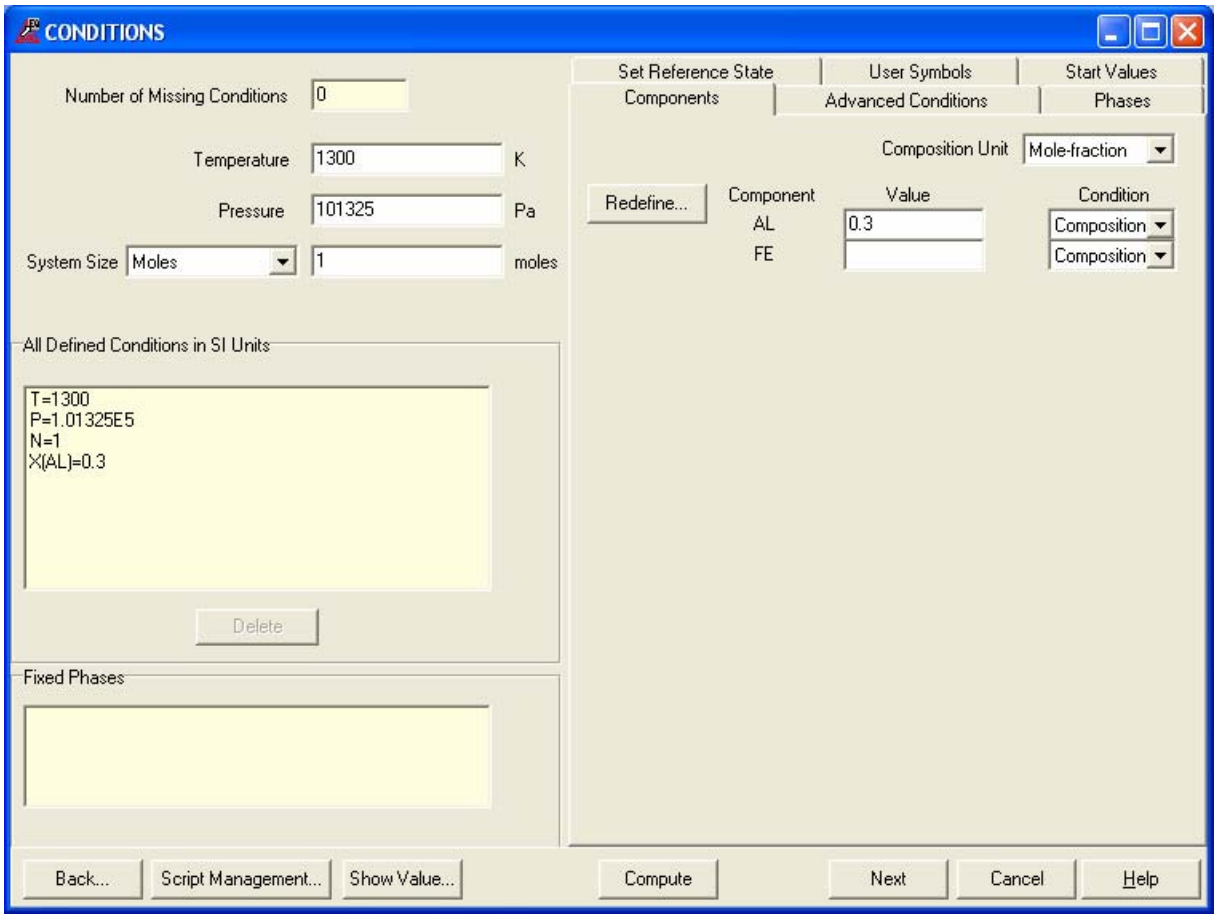
8. To plot the transition line in the Al-Fe phase diagram save the plot on an experimental file (e.g. example9.exp).



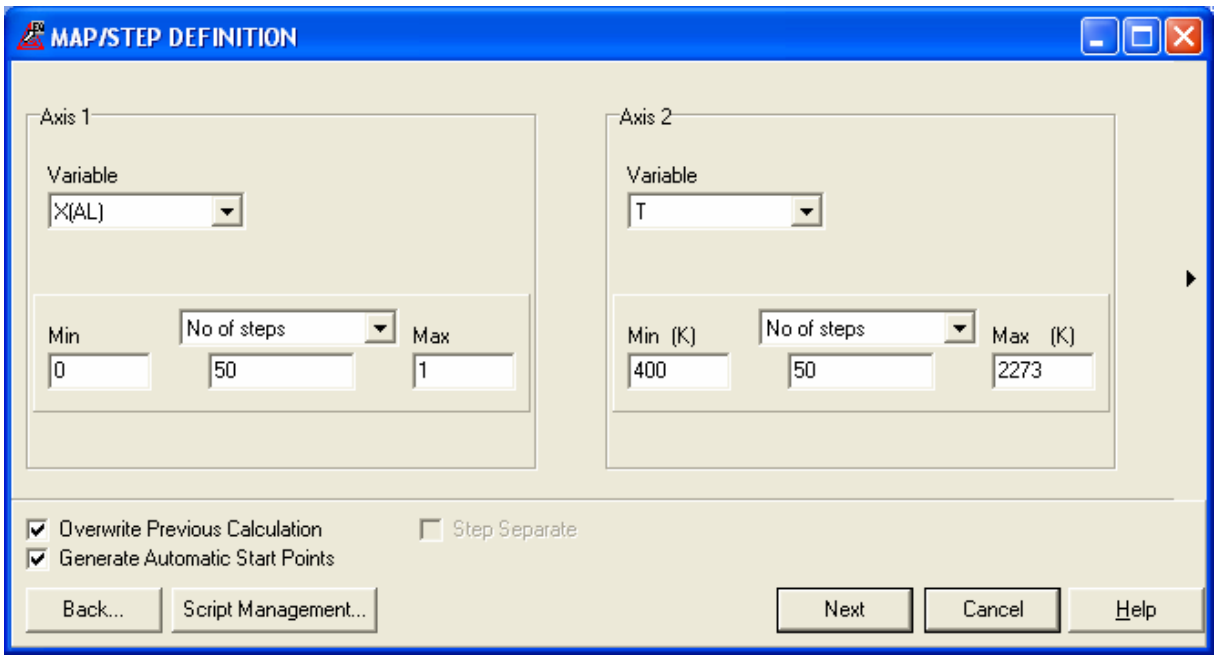
9. Close the GRAPH window and select *Elements* in the MAIN window. Reject all phases and select *LIQUID, FCC_A1, B2_BCC, BCC_A2, A2_BCC, AL13FE4, AL2FE, AL5FE2 and AL5FE4*. Finally, click *Next*.



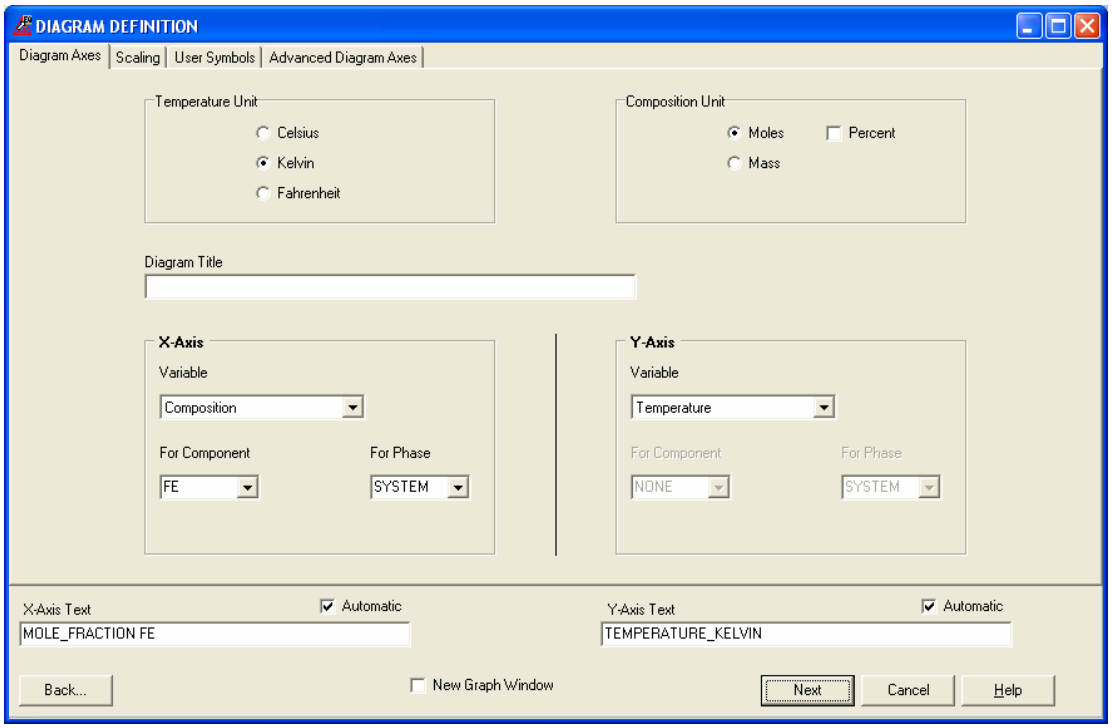
10. Enter T=1300 K and X(AL)=0.3. Click *Next.*

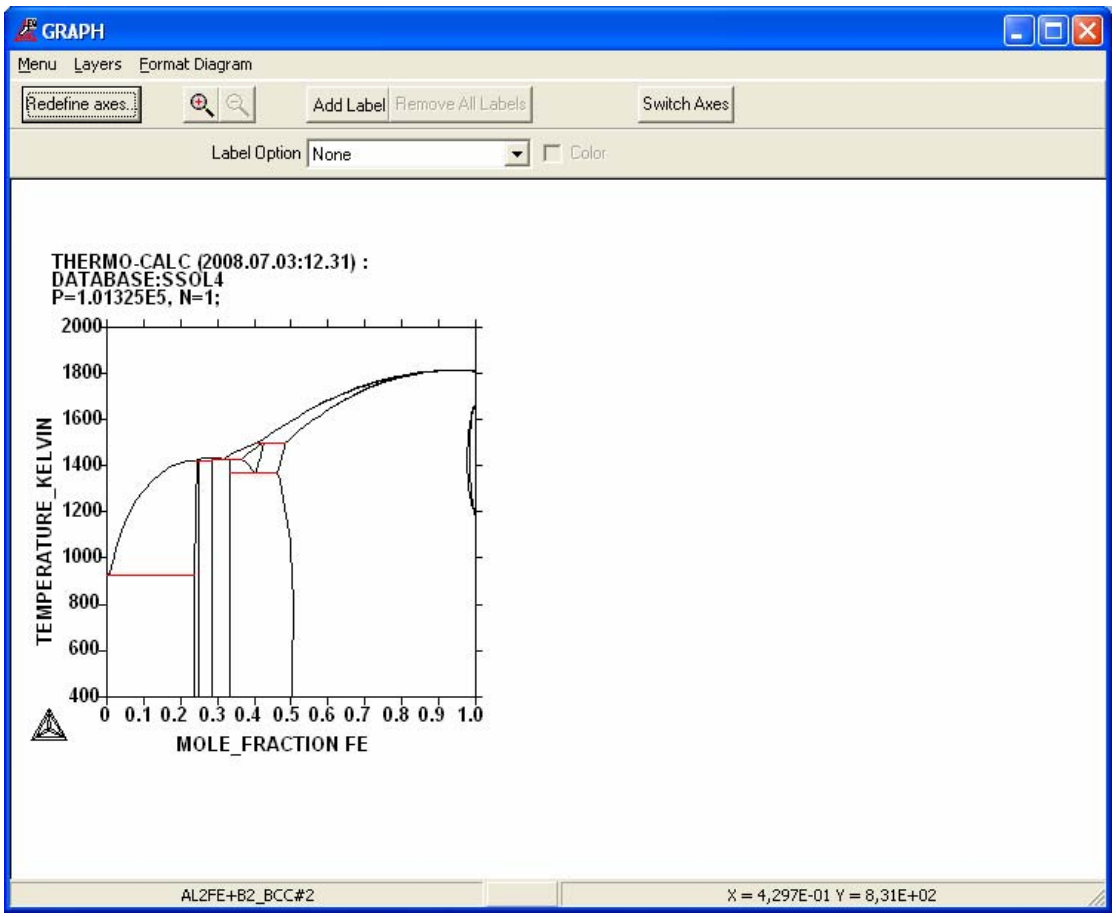


11. Set X(AL) as axis variable for x-axis and T as axis variable for y-axis and click *Next* to map the phase diagram.

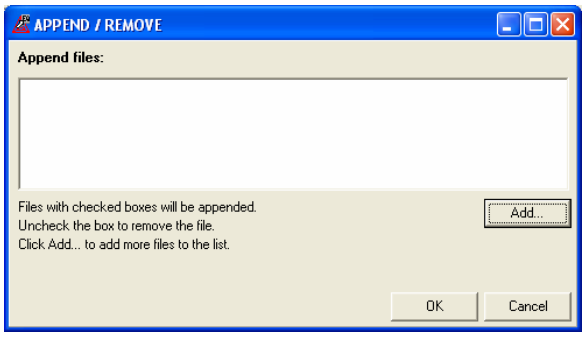


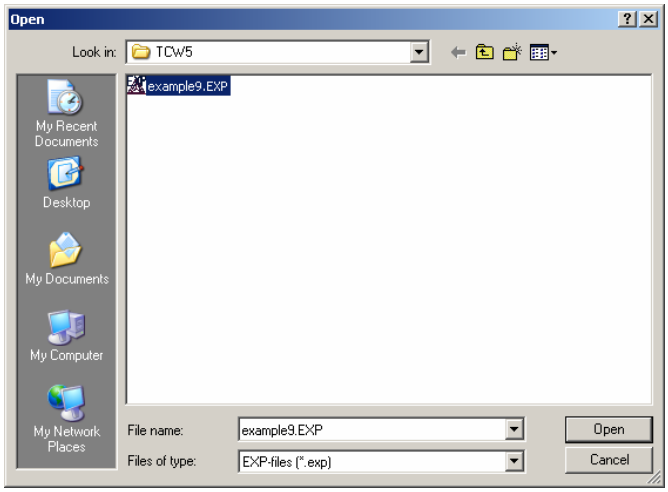
12. Select *Mole Fraction* of *Fe* and *Temperature* as diagram axes and click *Next* to plot.

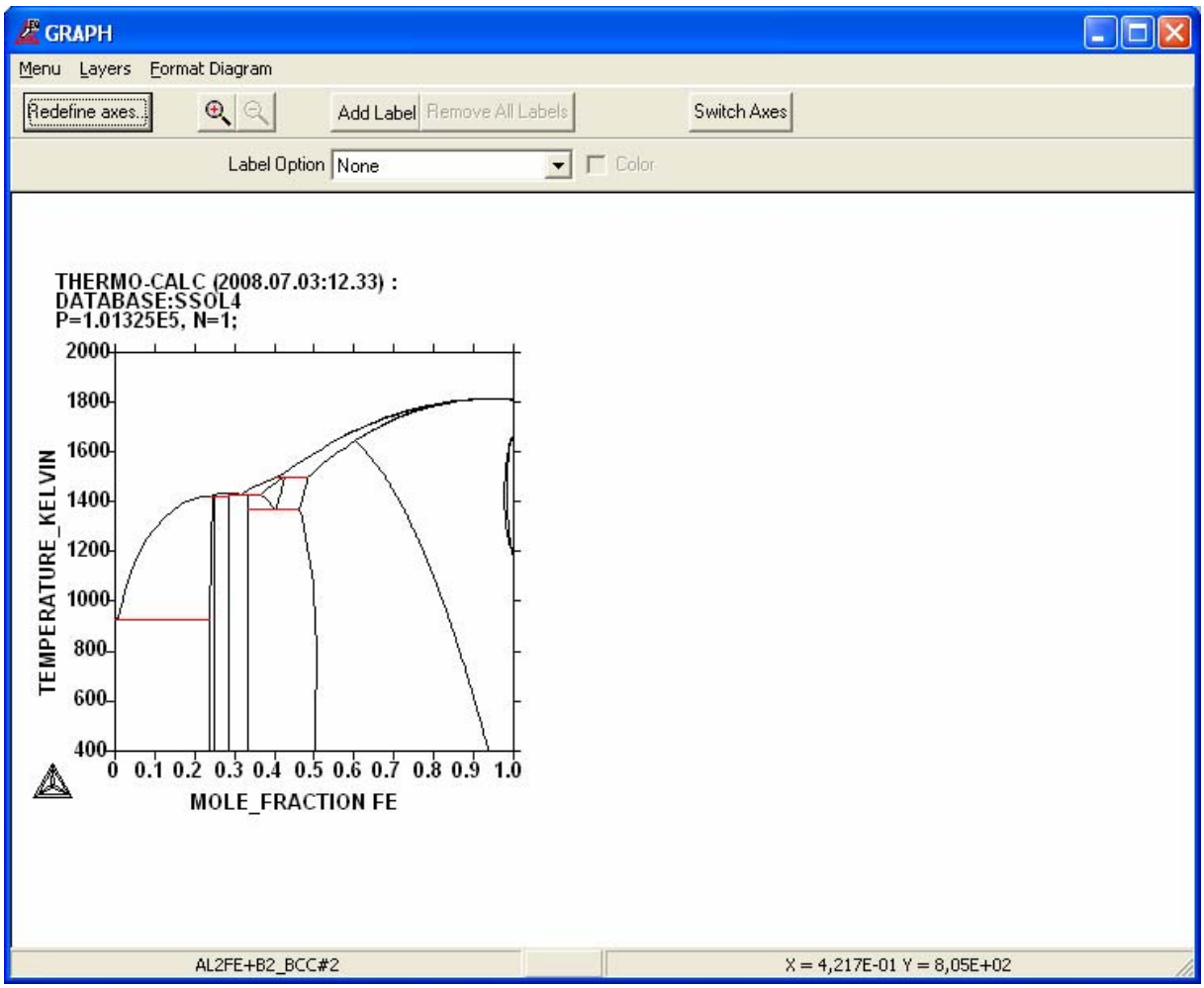




13. To plot the transition line in the phase diagram select *Append* under *Menu* and find the experimental plot file created earlier (example9.EXP).


APPEND / REMOVE
Append files:
Files with checked boxes will be appended.
Uncheck the box to remove the file.
Click Add... to add more files to the list.
Add...
OK
Cancel


Open
Look in:
TCW5
example9.EXP
My Recent Documents
Desktop
My Documents
My Computer
My Network Places
File name:
example9.EXP
Files of type:
EXP-files (*.exp)
Open
Cancel

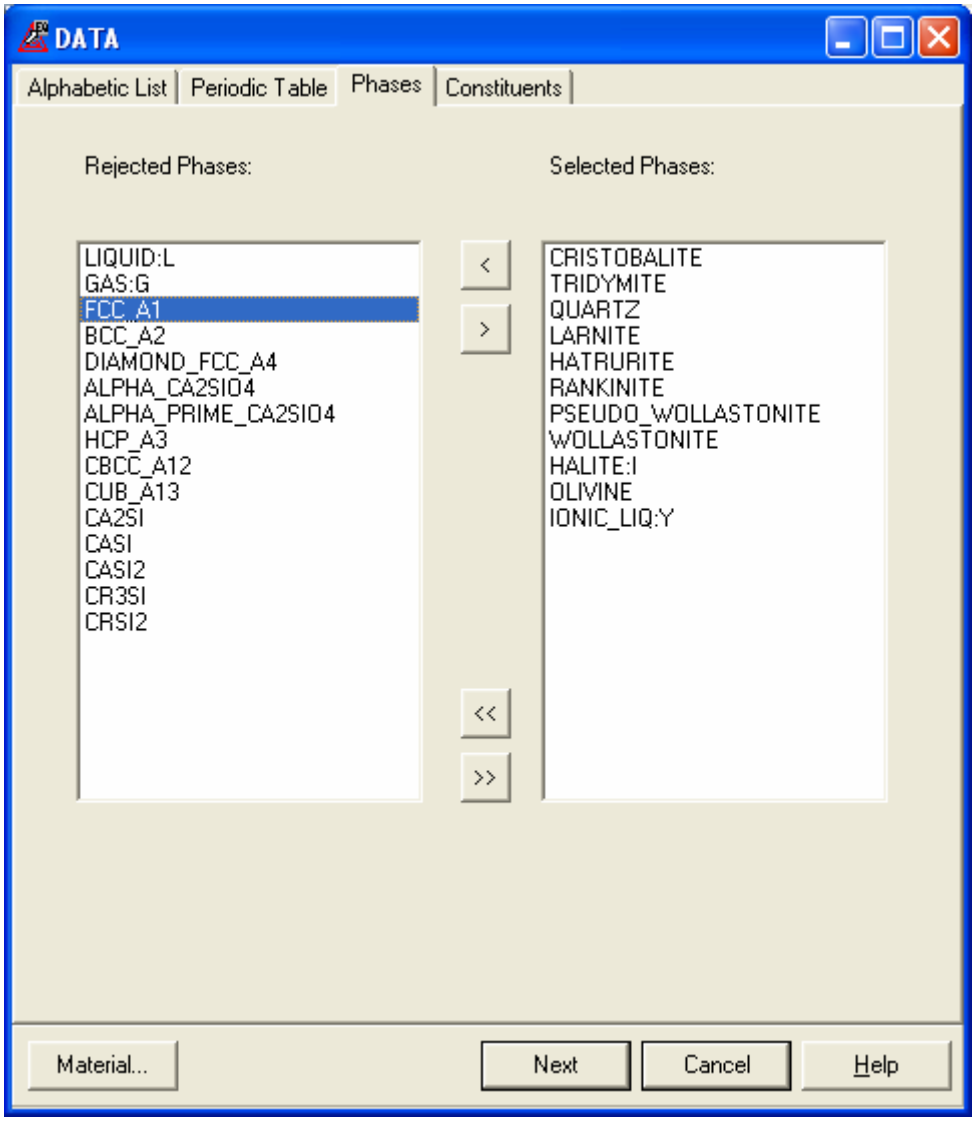

GRAPH
Menu
Layers
Format Diagram
Redefine axes...
Add Label
Remove All Labels
Switch Axes
Label Option
None
Color
THERMO-CALC (2008.07.03:12.33) :
DATABASE:SSOL4
P=1.01325E5, N=1;
TEMPERATURE_KELVIN
2000
1800
1600
1400
1200
1000
800
600
400
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
MOLE_FRACTION FE
AL2FE+B2_BCC#2
X = 4,217E-01 Y = 8,05E+02

10 Calculate the CaO-SiO2 System

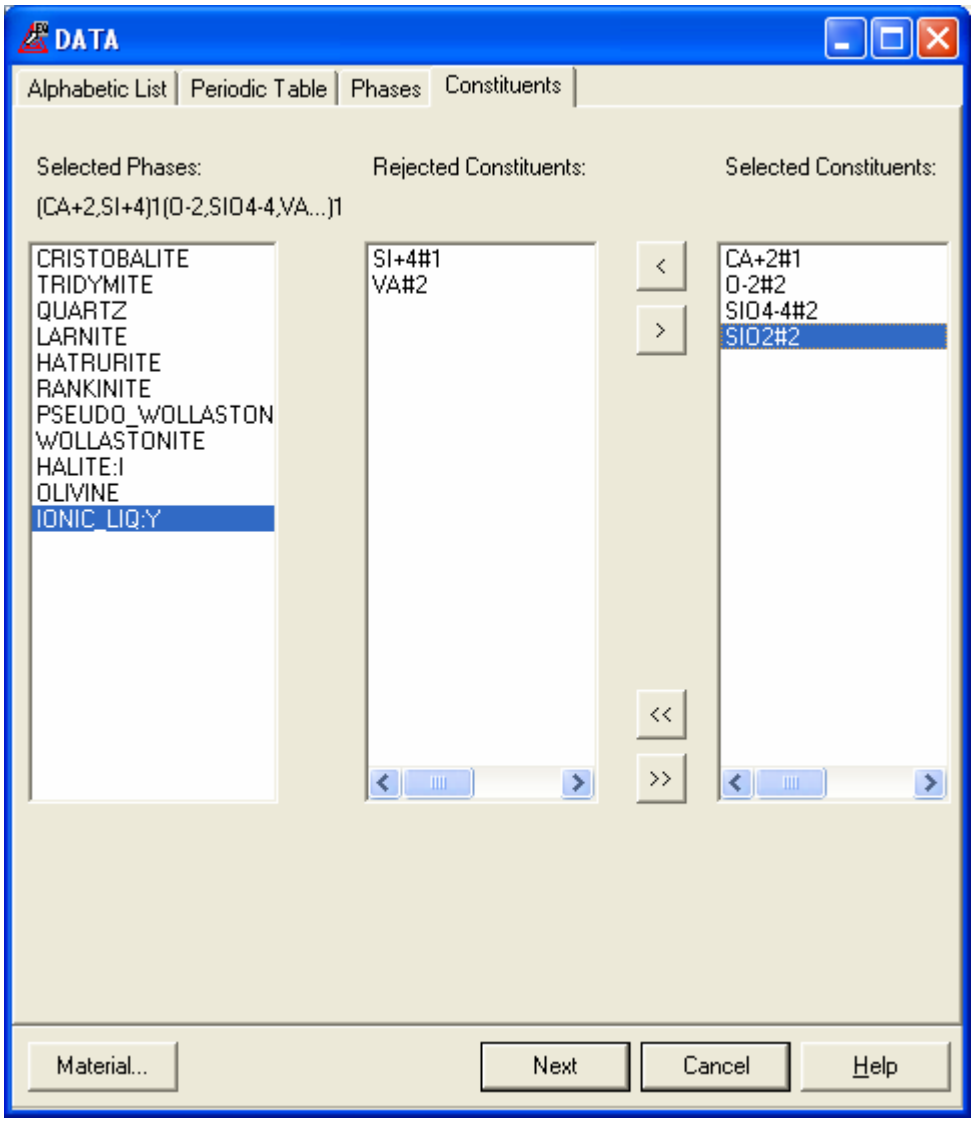
1. Click the *Elements* button in the MAIN window.

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.

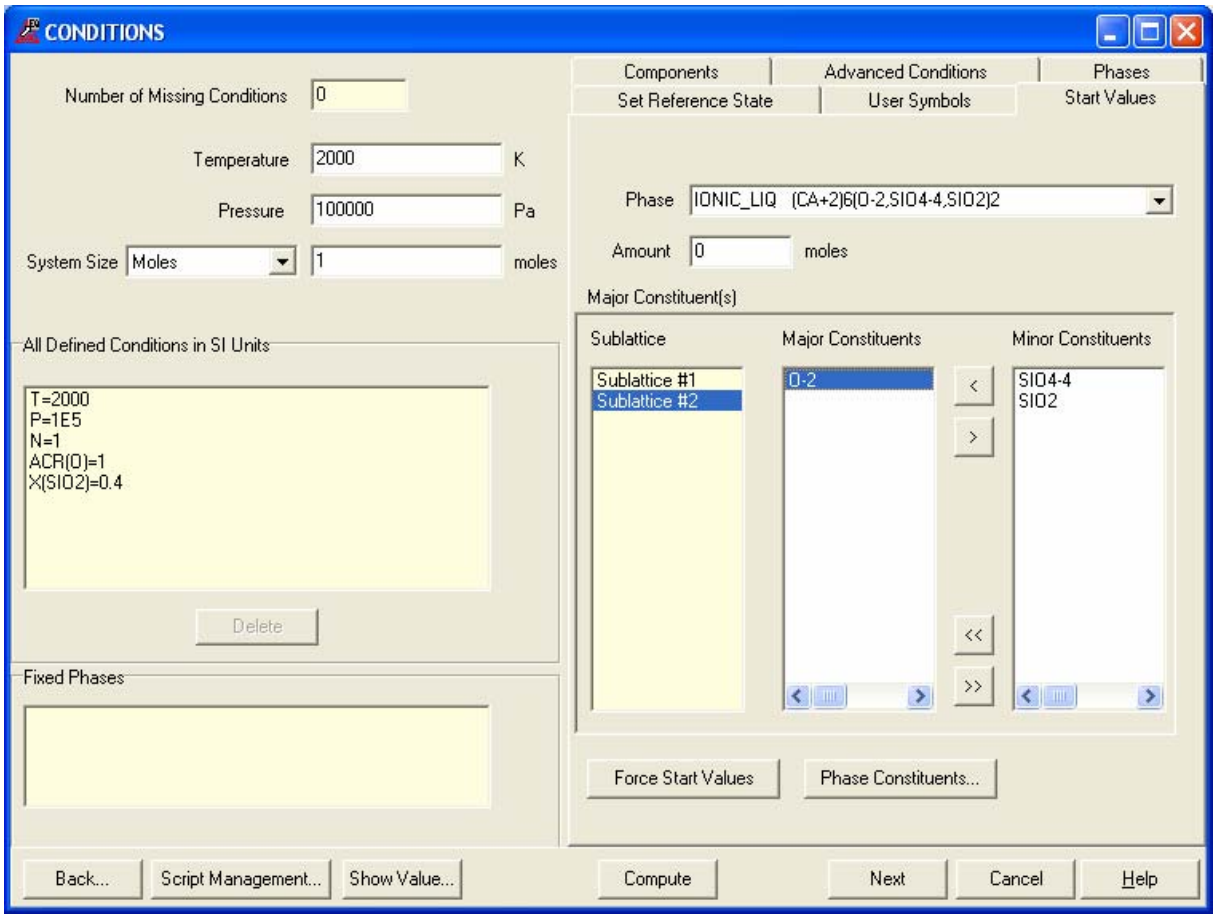


4. Next, reject the following constituents from the IONIC_LIQ:Y phase: VA#2 and SI+4#1.



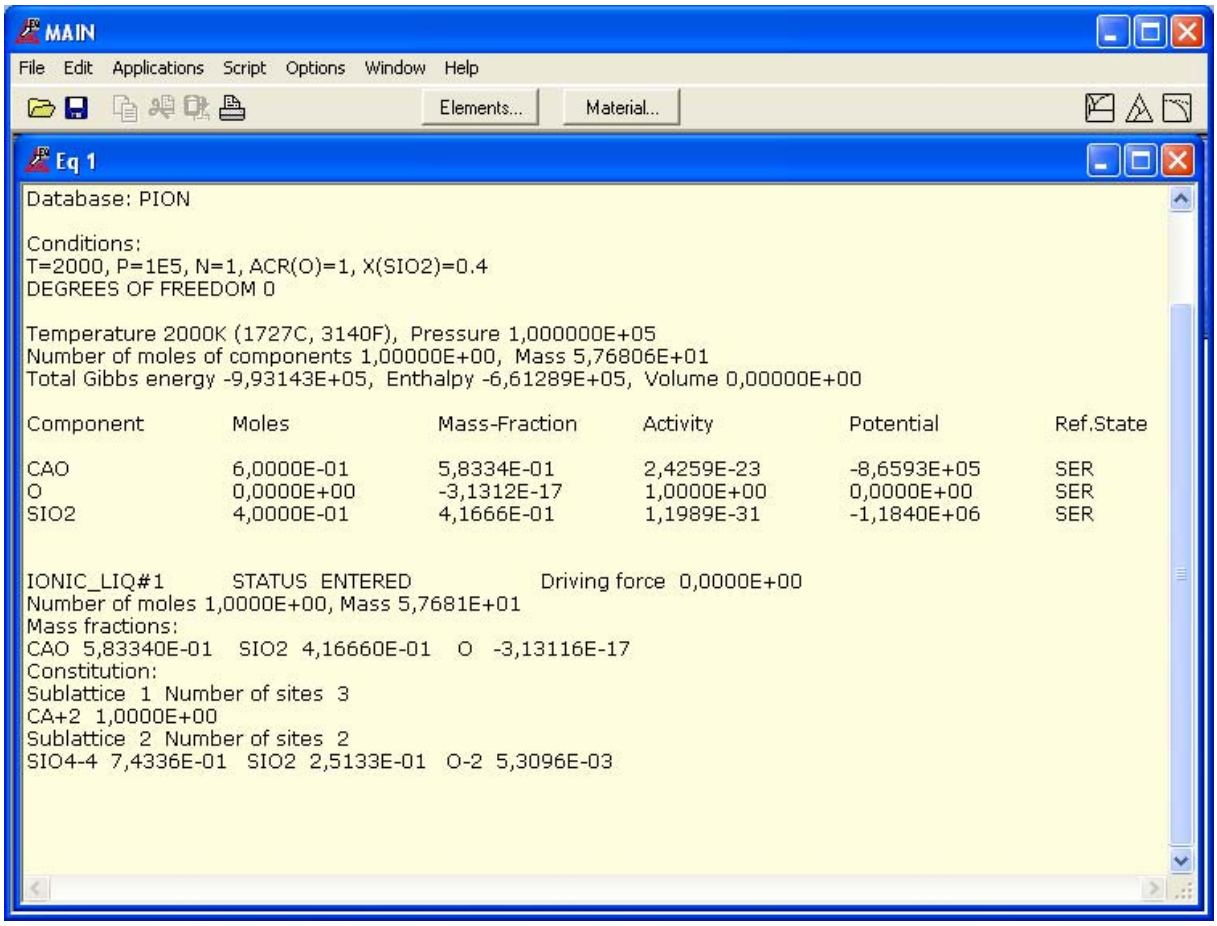
5. Click *Next* to come to the CONDITIONS window**.** Define more convenient components than the elements. Click *Redefine* and enter *CAO*, *SIO2* and *O*. Click *Ok* to return to the CONDITIONS window.

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.



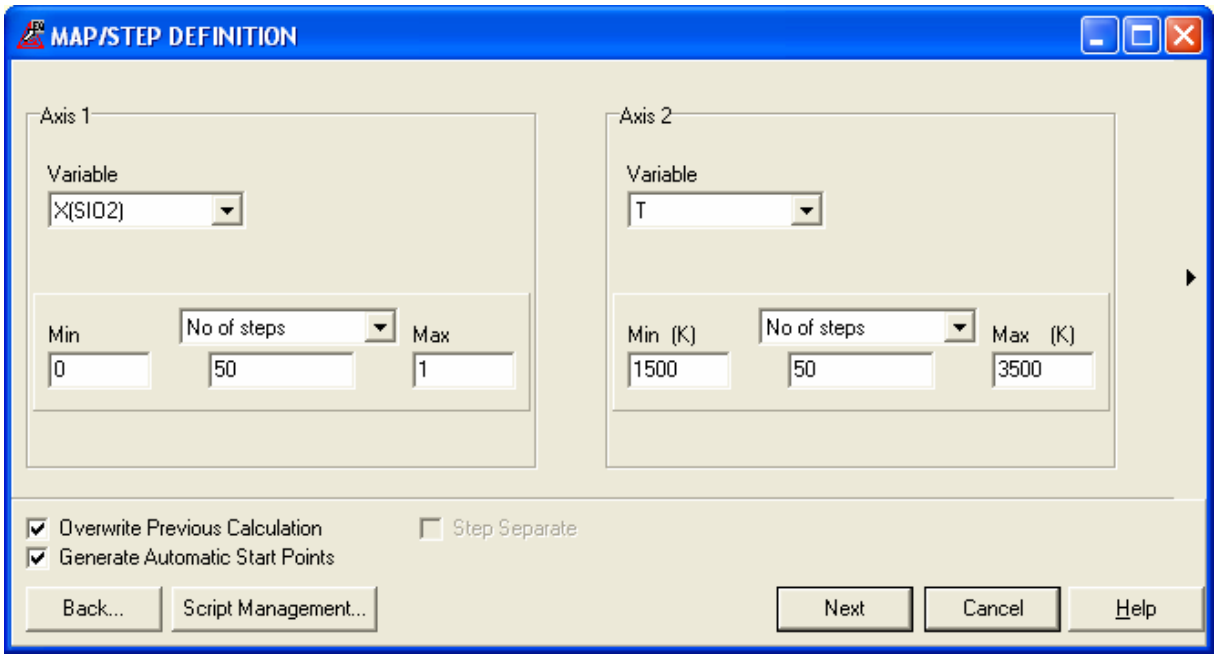
7. Click *Start Values* tab and change the major constituent in sublattice 2 in IONIC_LIQ to O-2.

8. Click *Compute* to perform an equilibrium calculation for the given conditions.



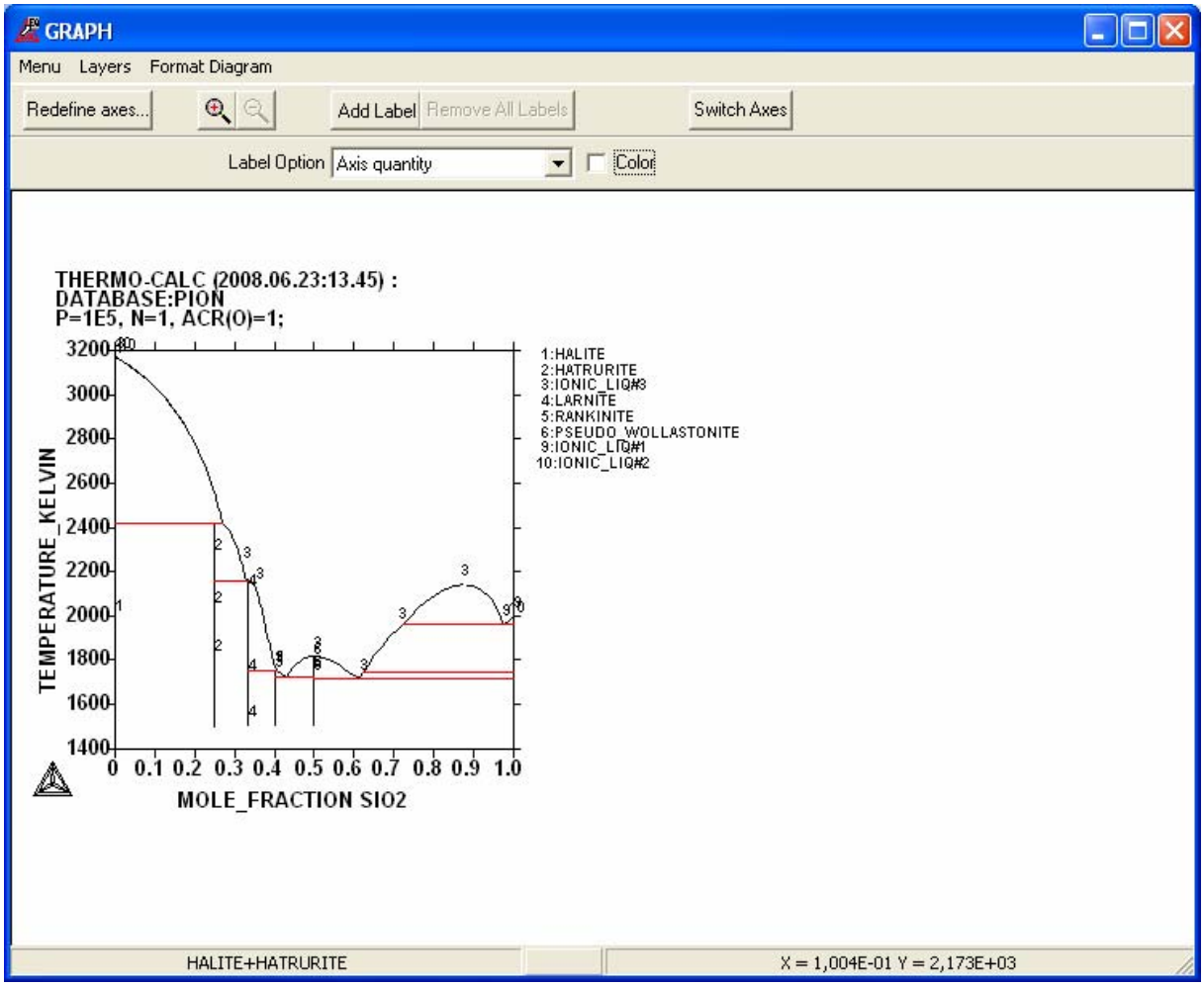
9. Click *Next* to come to the MAP/STEP DEFINITION window.

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. .

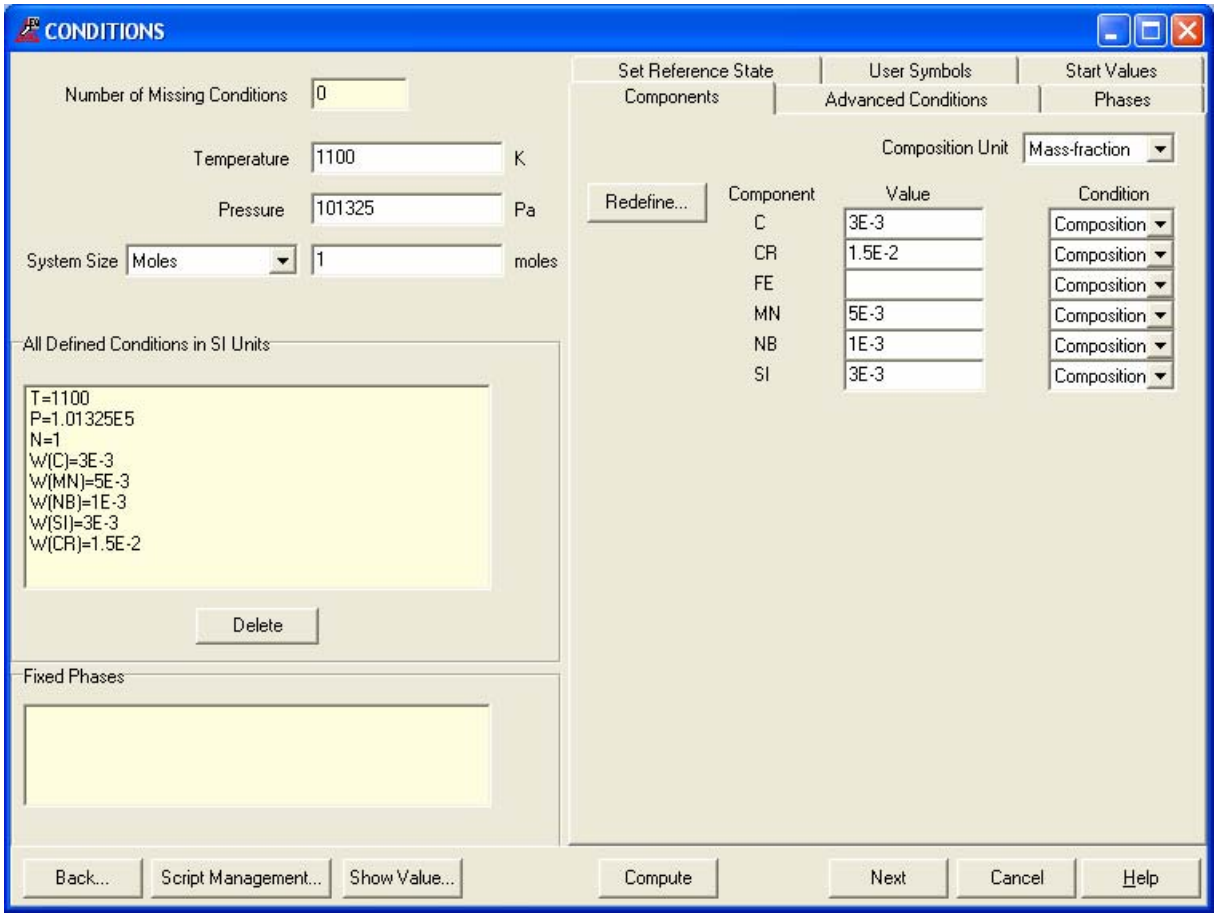


11 Calculate A3 Temperature and Its Dependence on Alloying Element

1. Click the *Elements* button in the MAIN window.

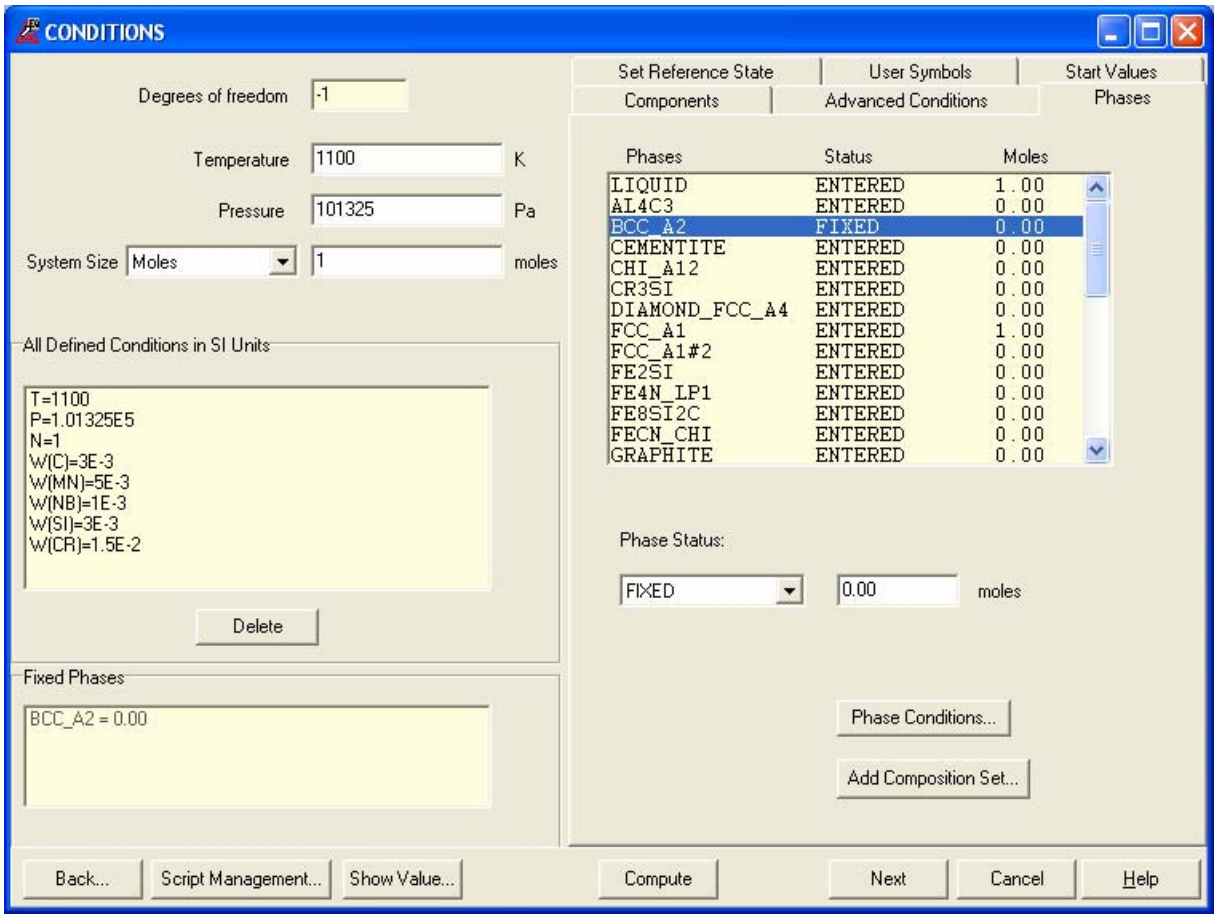
2. Select database *TCFE6* and elements *C*, *Cr, Fe, Mn, Nb* and *Si* from the periodic table.

3. Click *Next* to come to the CONDITIONS window. Enter compositions in mass-fraction and the temperature: W(Cr)=1.5E-2, W(C)=3E-3, W(Mn)=5E-3, W(Nb)=1E-3, W(Si)=3E-3, T=1100 K.



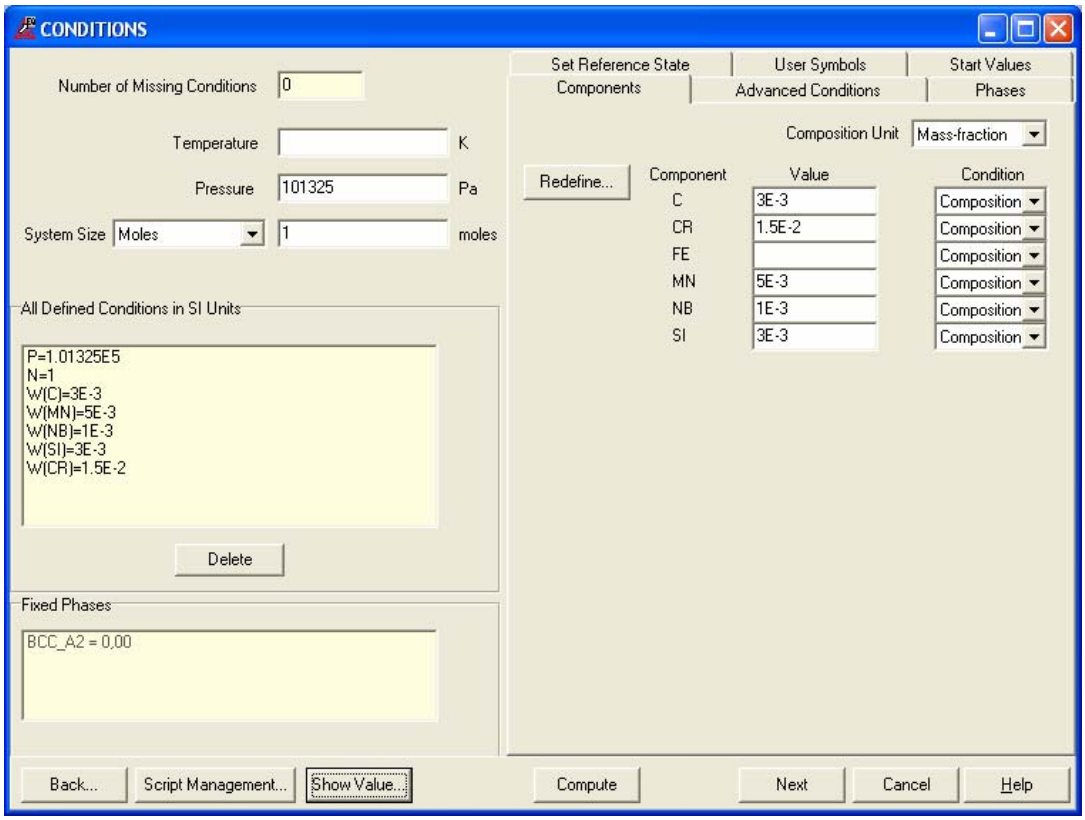
4. Click *Compute* to perform an equilibrium calculation for the given conditions.

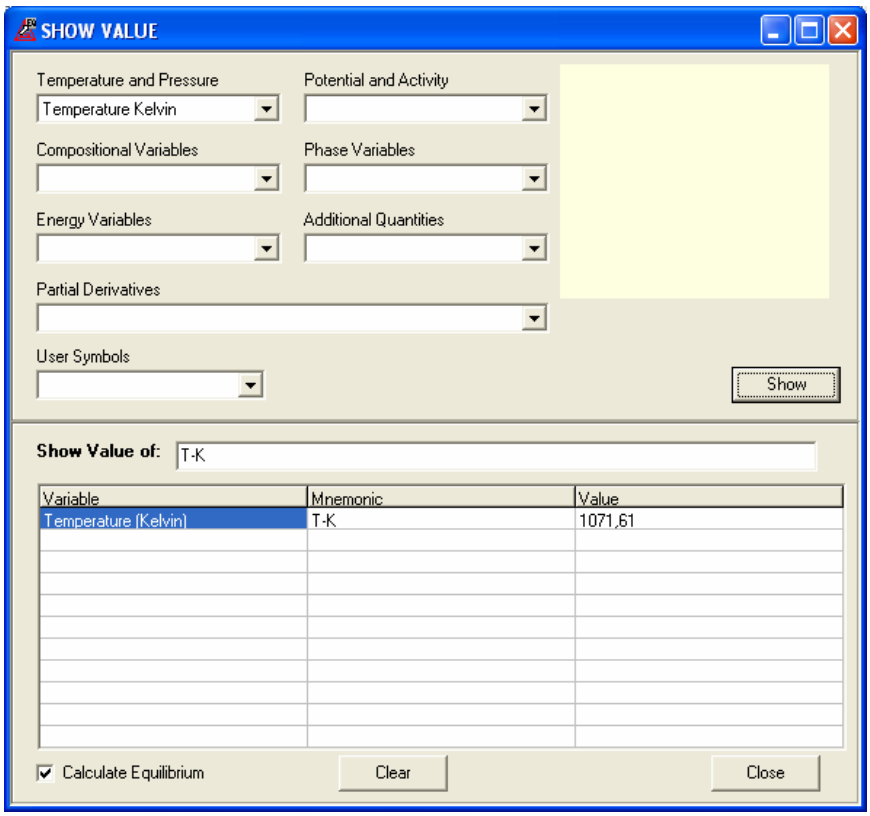
5. Fix the BCC_A2 phase with zero moles and remove the temperature condition.



6. Click *Compute* once more.

7. 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.





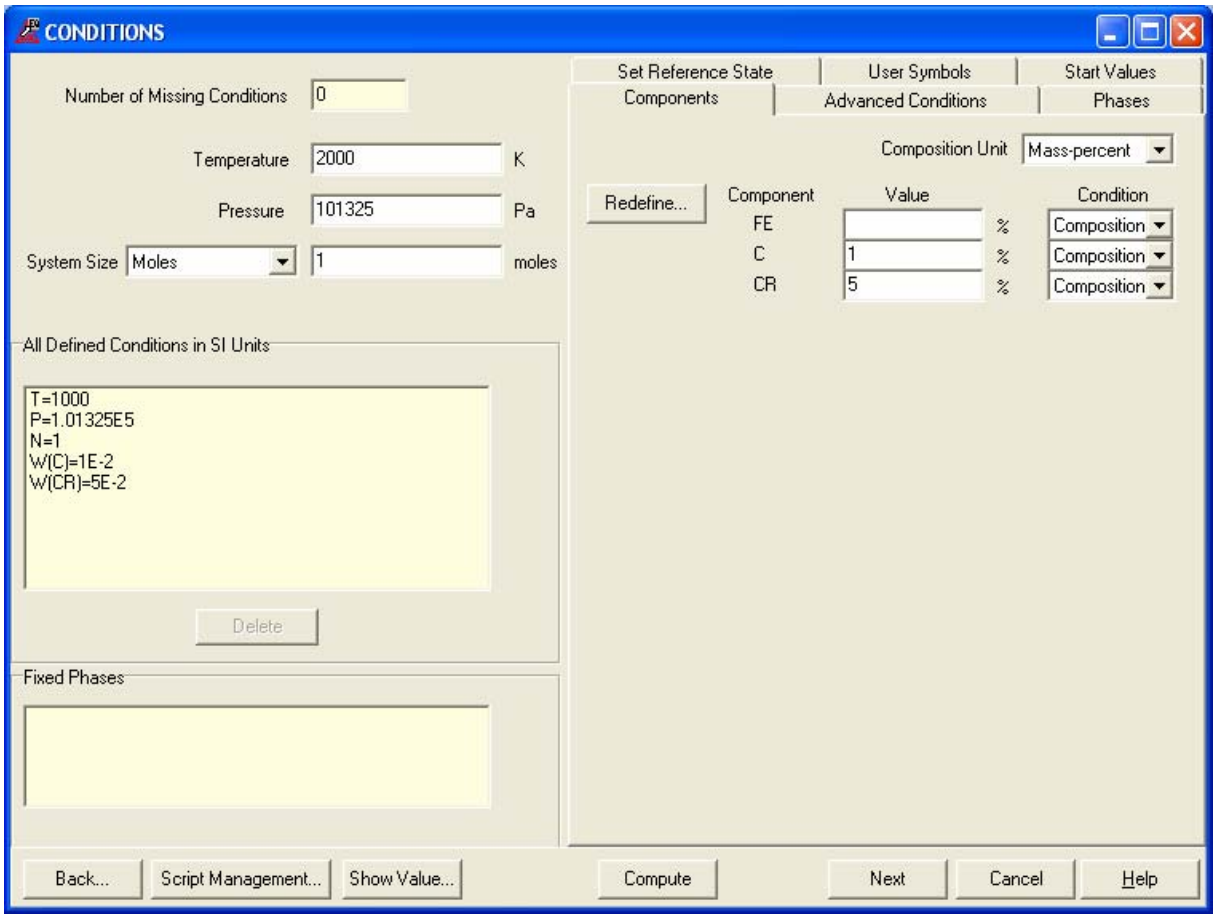
8. To investigate the dependence of the A_3 temperature on alloy composition, try changing one of the mass-fractions and click *Compute* after each change. Click *Show* in the SHOW VALUE window to see the new temperature.

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

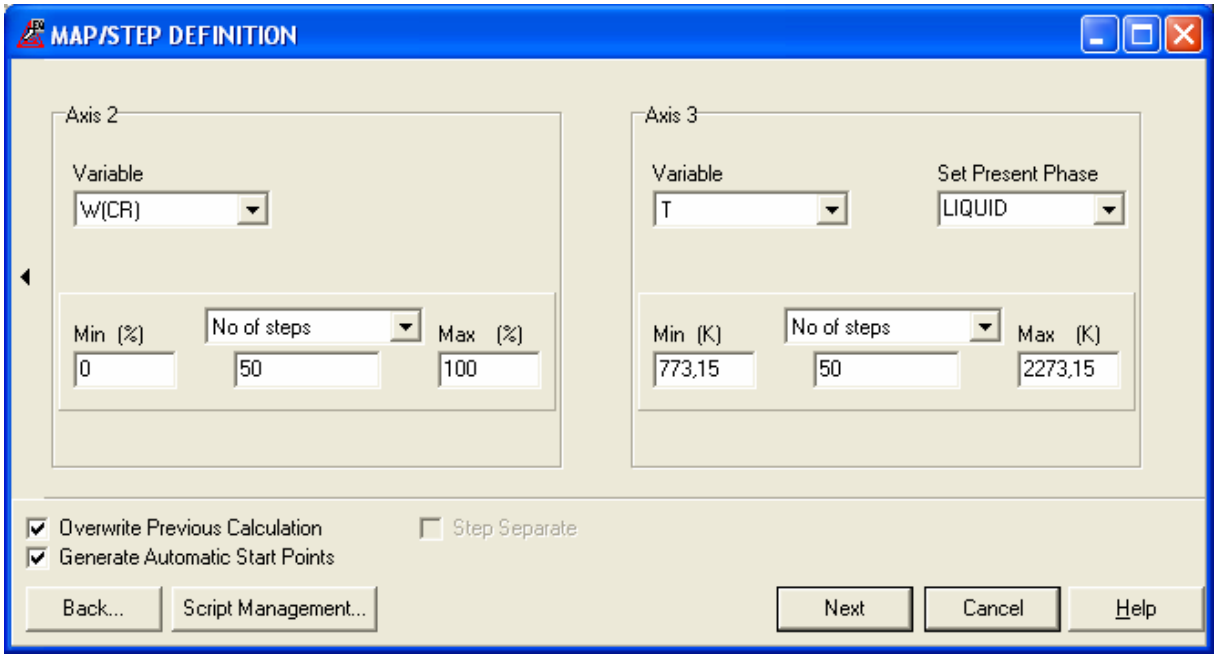
1. Click *Elements* in the MAIN window.

2. Select *PTERN* from the *Database* list and then click alloy elements *Fe*, *C*, and *Cr* in the periodic table. Click *Next*.

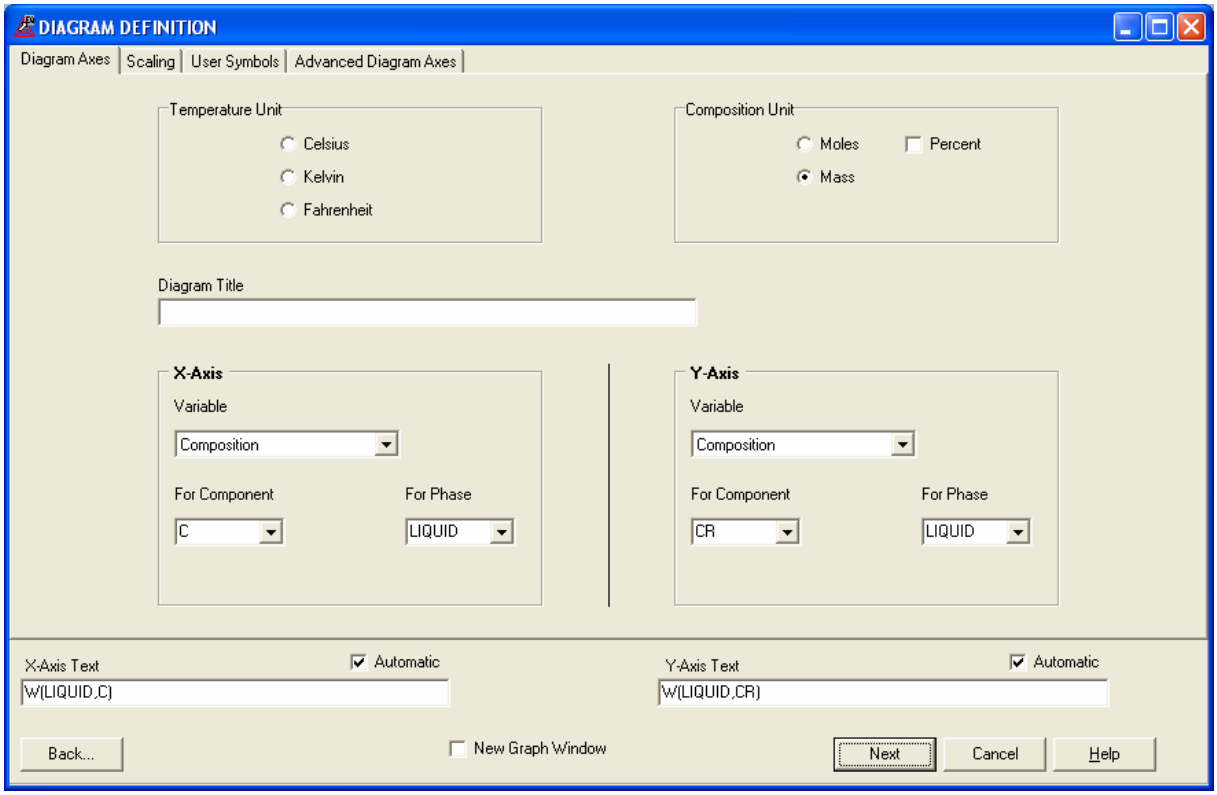
3. Specify the concentrations of C and Cr as *1* and *5 mass-percent*, respectively and change the temperature to *2000 K*. Click *Next*.



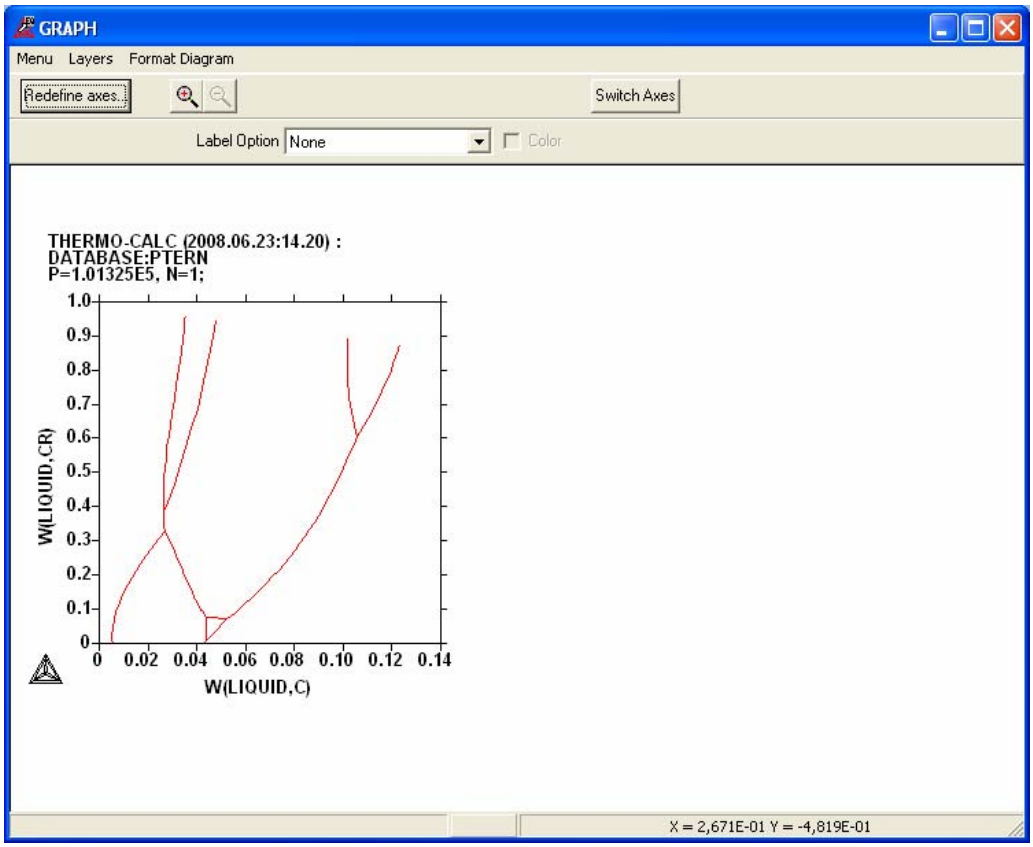
4. Set the variable for *Axis 1 to W(C)* and the variable for *Axis 2* to *W(CR)*. Click the arrow on the right of the window, and the panel for *Axis 3* appears. Choose *T* as the variable for the third axis and select *LIQUID* as the *Present Phase* since we are going to map the univariant equilibrium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



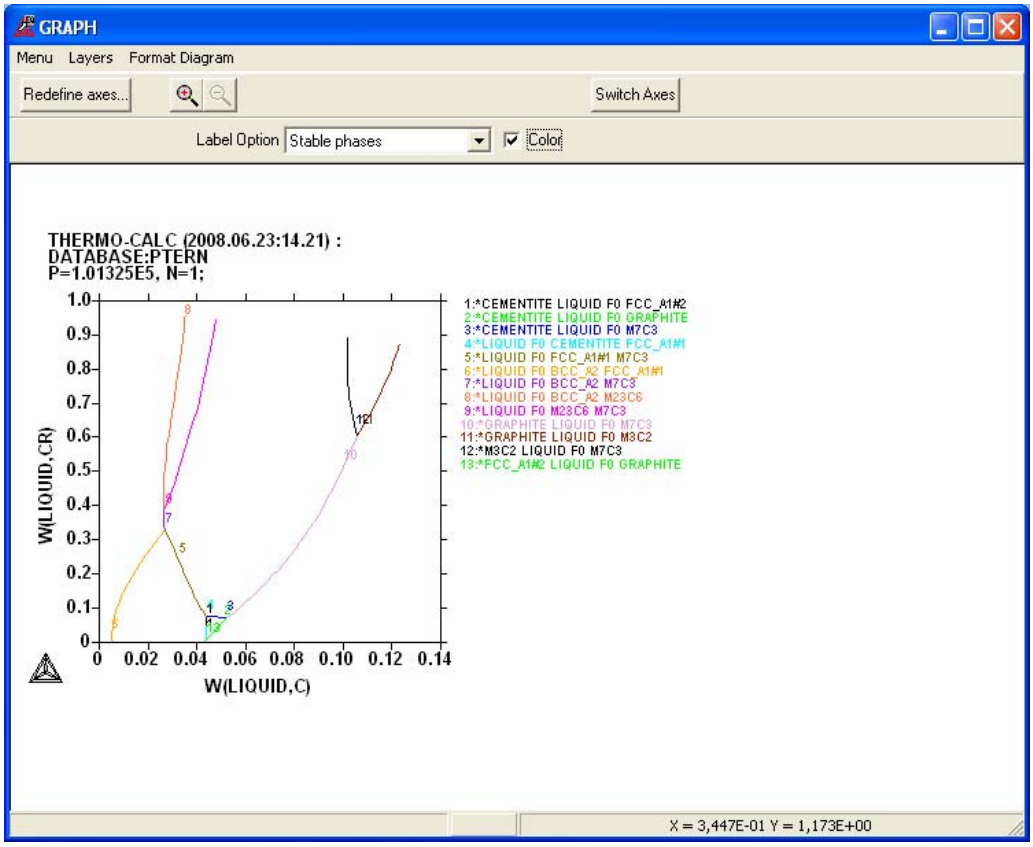
5. The default axes are mass-fraction of C and CR in the LIQUID phase. Accept this choice and click *Next*.



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



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

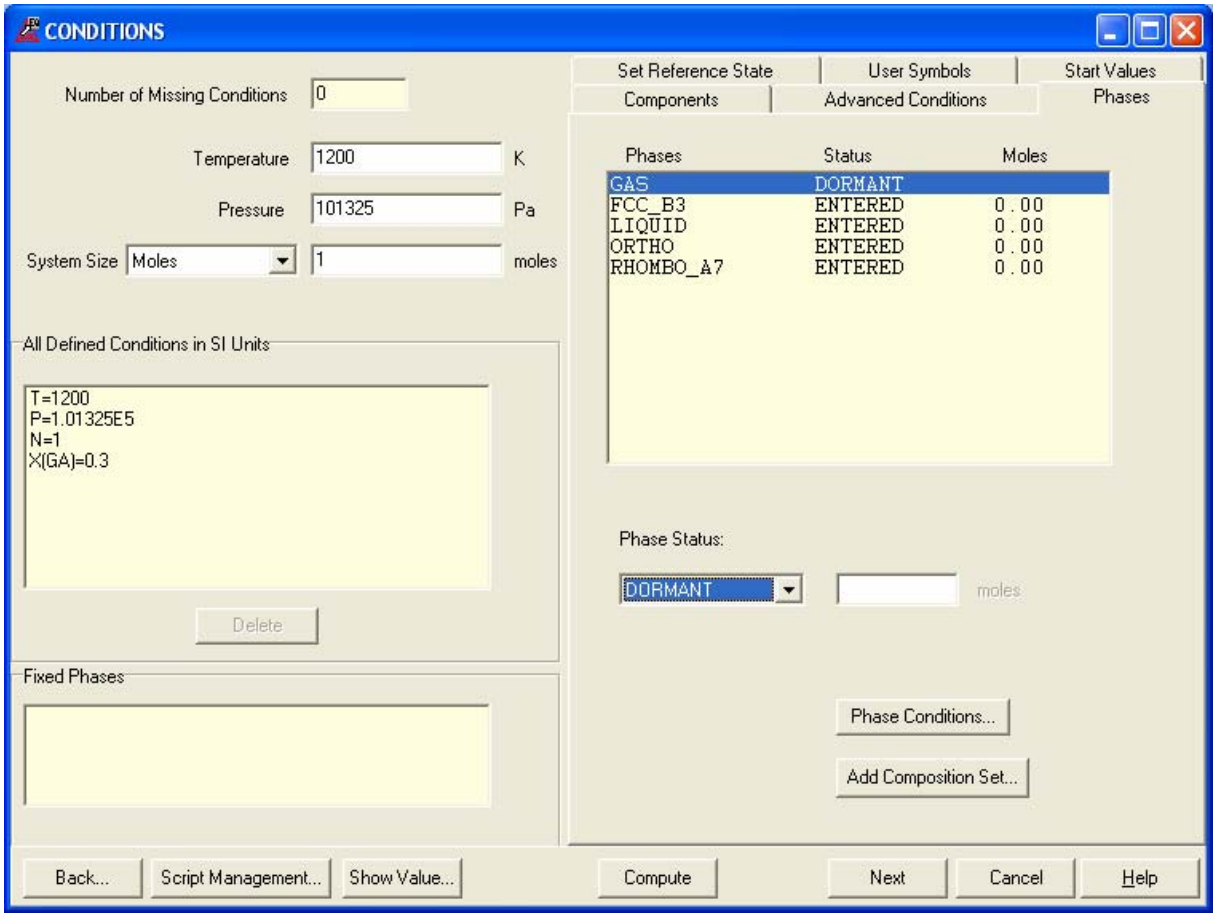


13 Plotting of Partial Pressure of Gas Species Along Solubility Lines in As-Ga Phase Diagram

1. Click Elements in the MAIN window. Select database *PG35* and elements *As* and *Ga* in the periodic system.

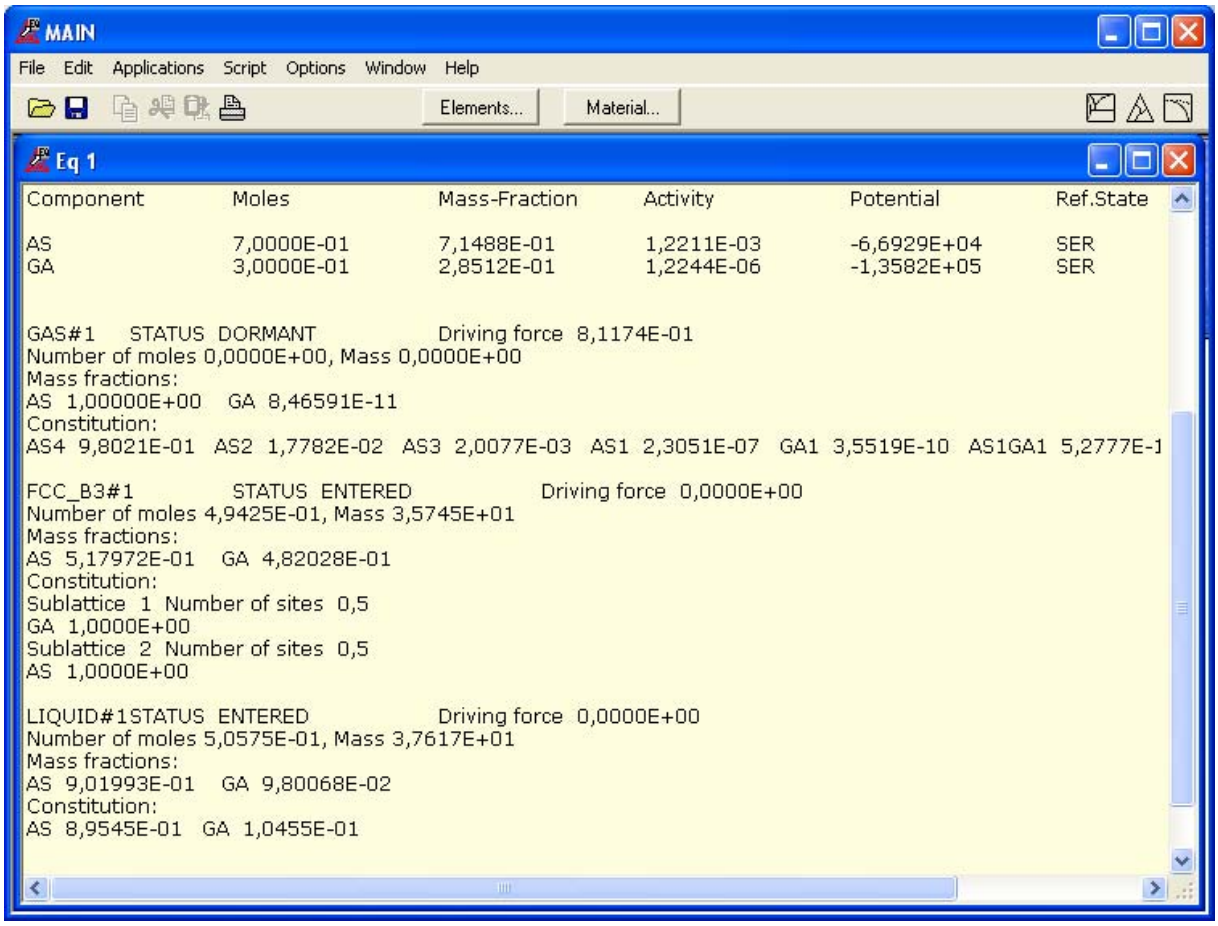
2. Reject all phases and select phases *LIQUID, RHOMBO_A7, ORTHO, FCC_B3* and *GAS*. Click *Next*.

3. Enter the conditions T=1200 K and X(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.

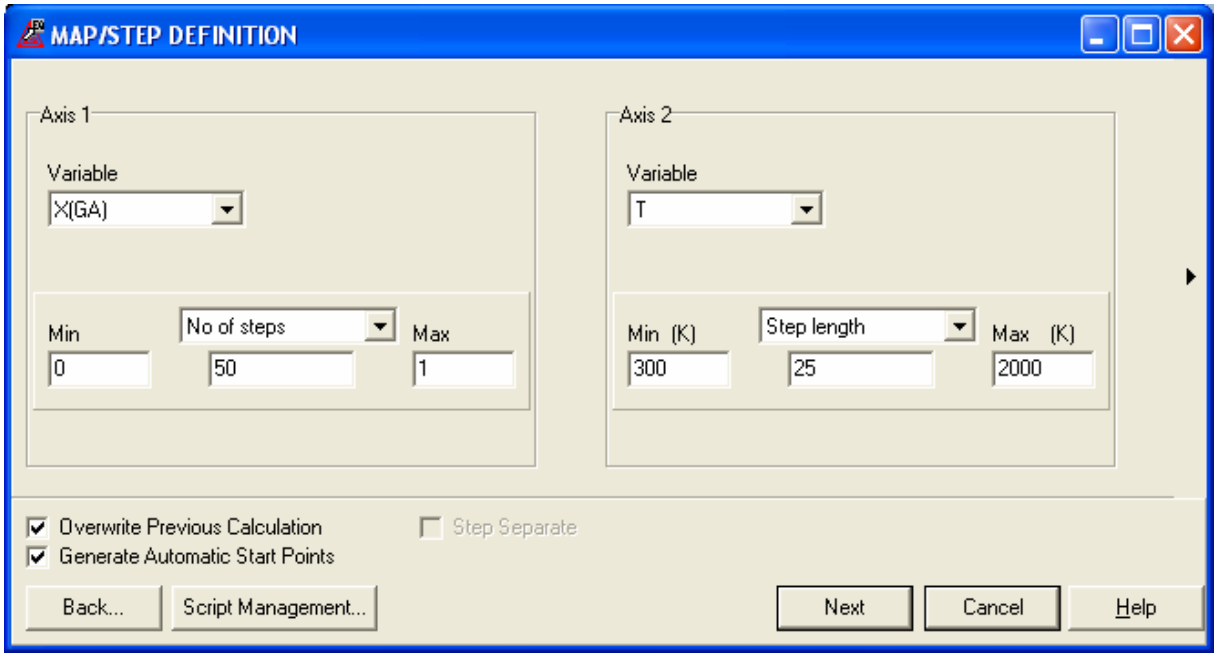


4. Click *Compute*.

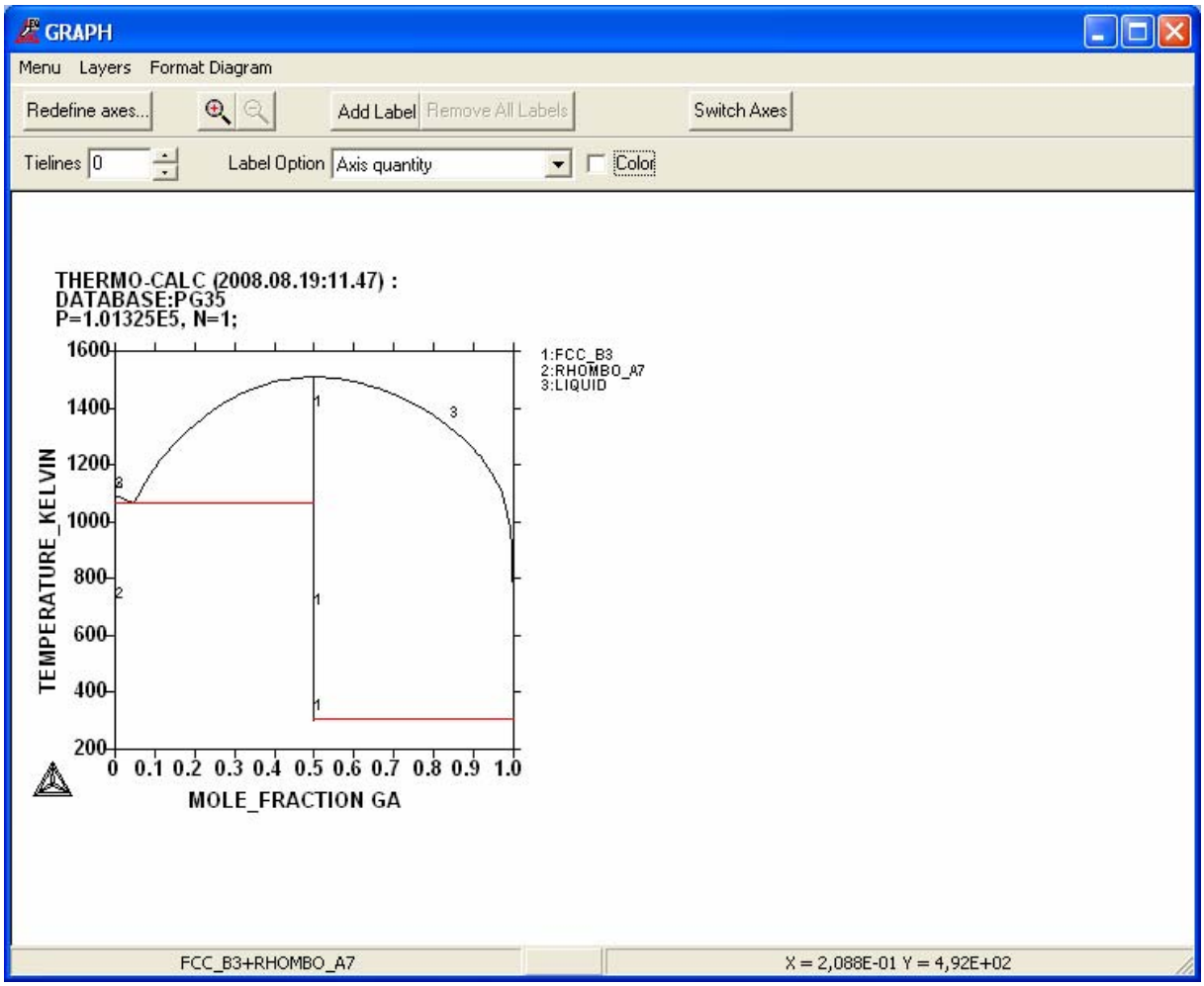
5. From the equilibrium calculation it can be seen that the GAS phase would like to be stable (positive driving force) but it is not allowed to form as it is dormant. Click *Next*.



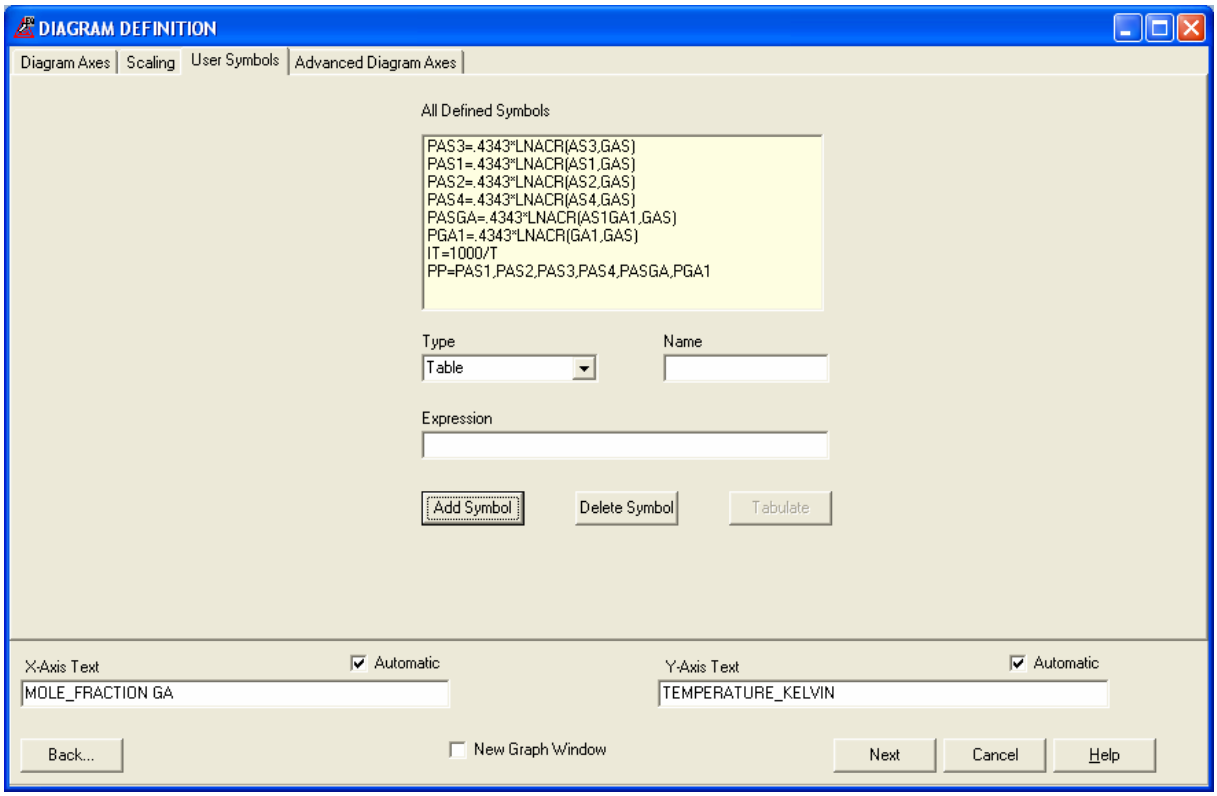
6. To map the phase diagram set X(GA) with range 0 to 1 and T with range 300 to 2000 (step length 25) as axis variables. Click *Next* to map.



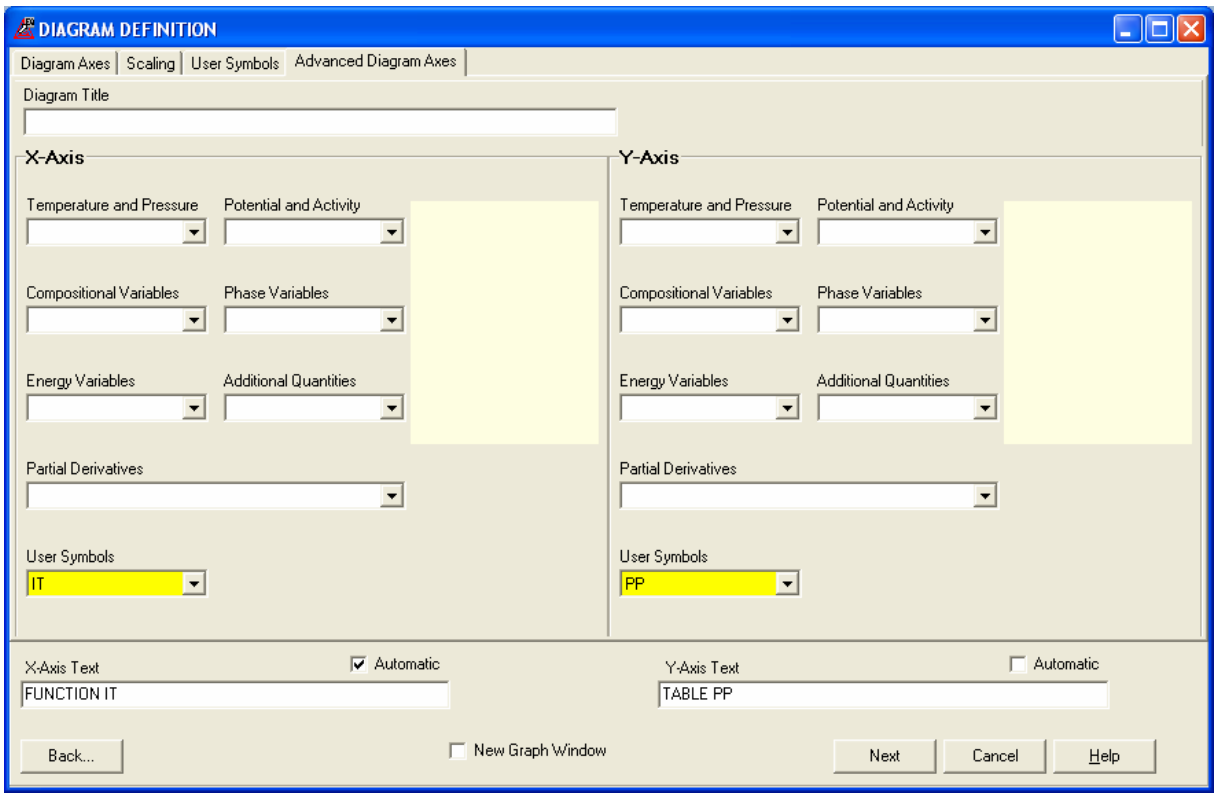
7. Accept the default diagram axes. Click *Next* to plot the As-Ga phase diagram.

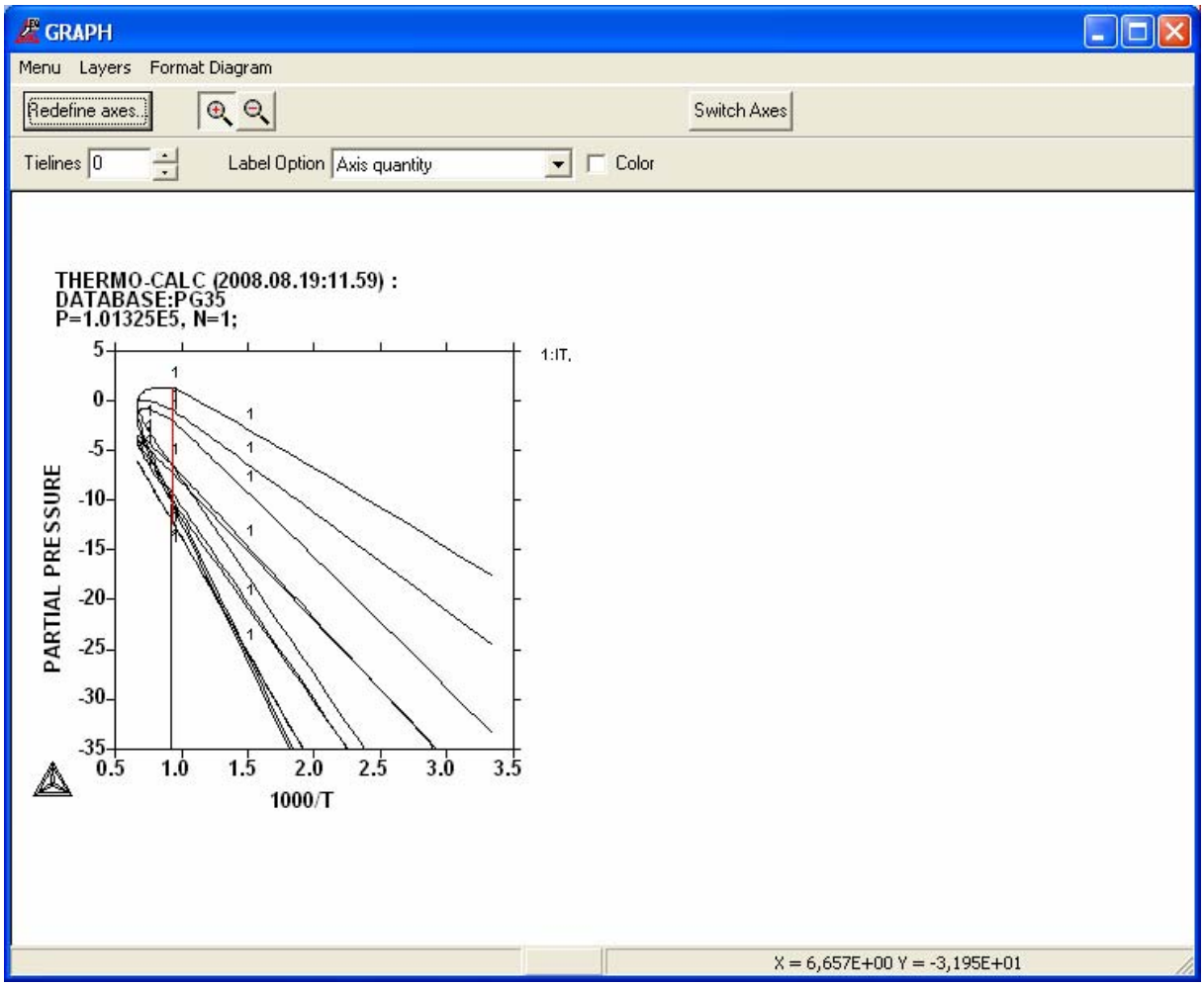


8. Now, one may be interested to know the partial pressures of the different gas species along the solubility lines. Click *Redefine* to return to the DIAGRAM DEFINITION window. Click the *User Symbols* tab and enter a number of functions and collect these in a table (see below).



9. 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.



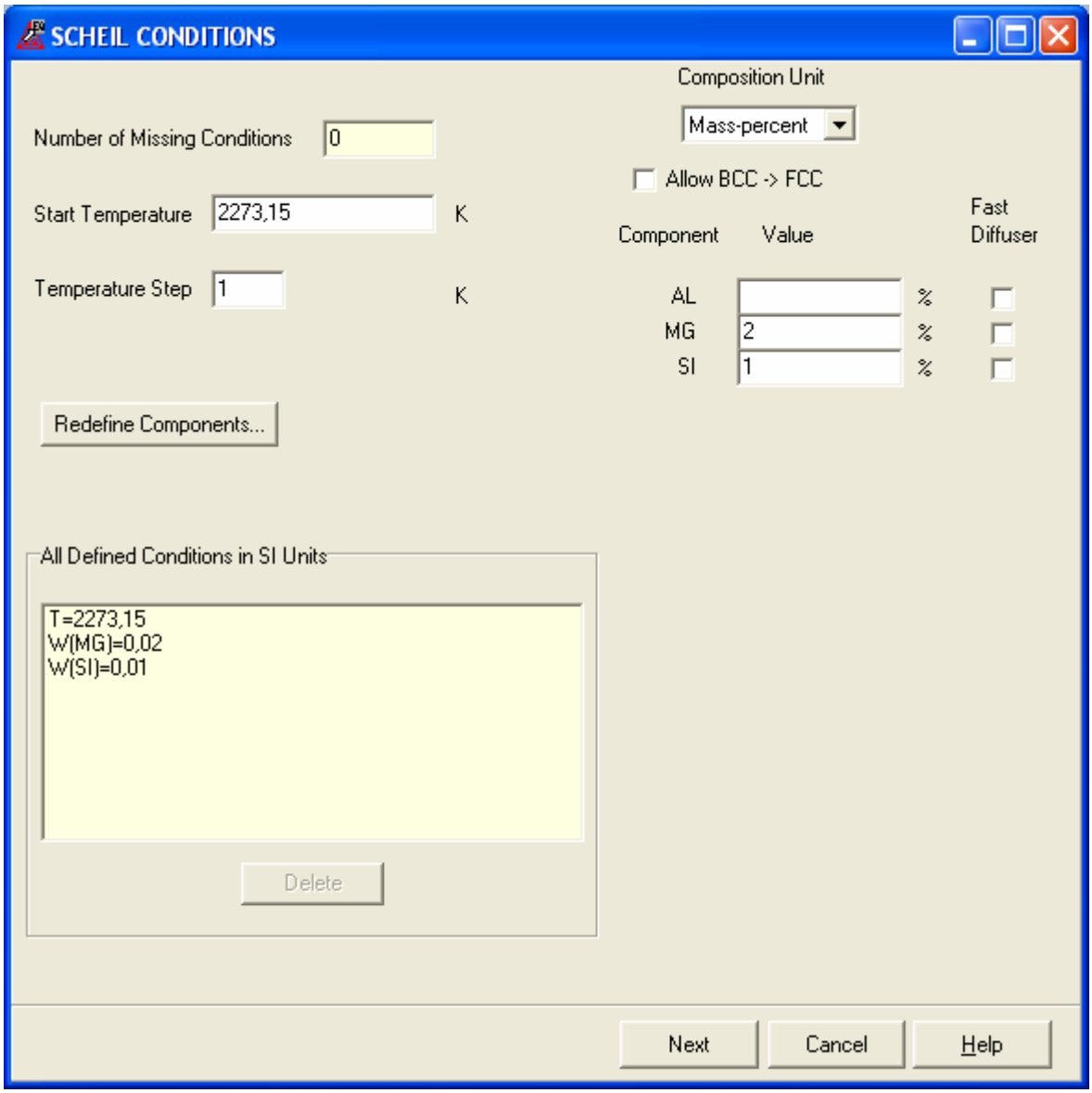

GRAPH
Menu Layers Format Diagram
Redefine axes...
Switch Axes
Tielines 0
Label Option Axis quantity
Color
THERMO-CALC (2008.08.19:11.59) :
DATABASE:PG35
P=1.01325E5, N=1;
1:IT,
PARTIAL PRESSURE
1000/T
5
0
-5
-10
-15
-20
-25
-30
-35
0.5
1.0
1.5
2.0
2.5
3.0
3.5
X = 6,657E+00 Y = -3,195E+01

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

Click  in the MAIN window.

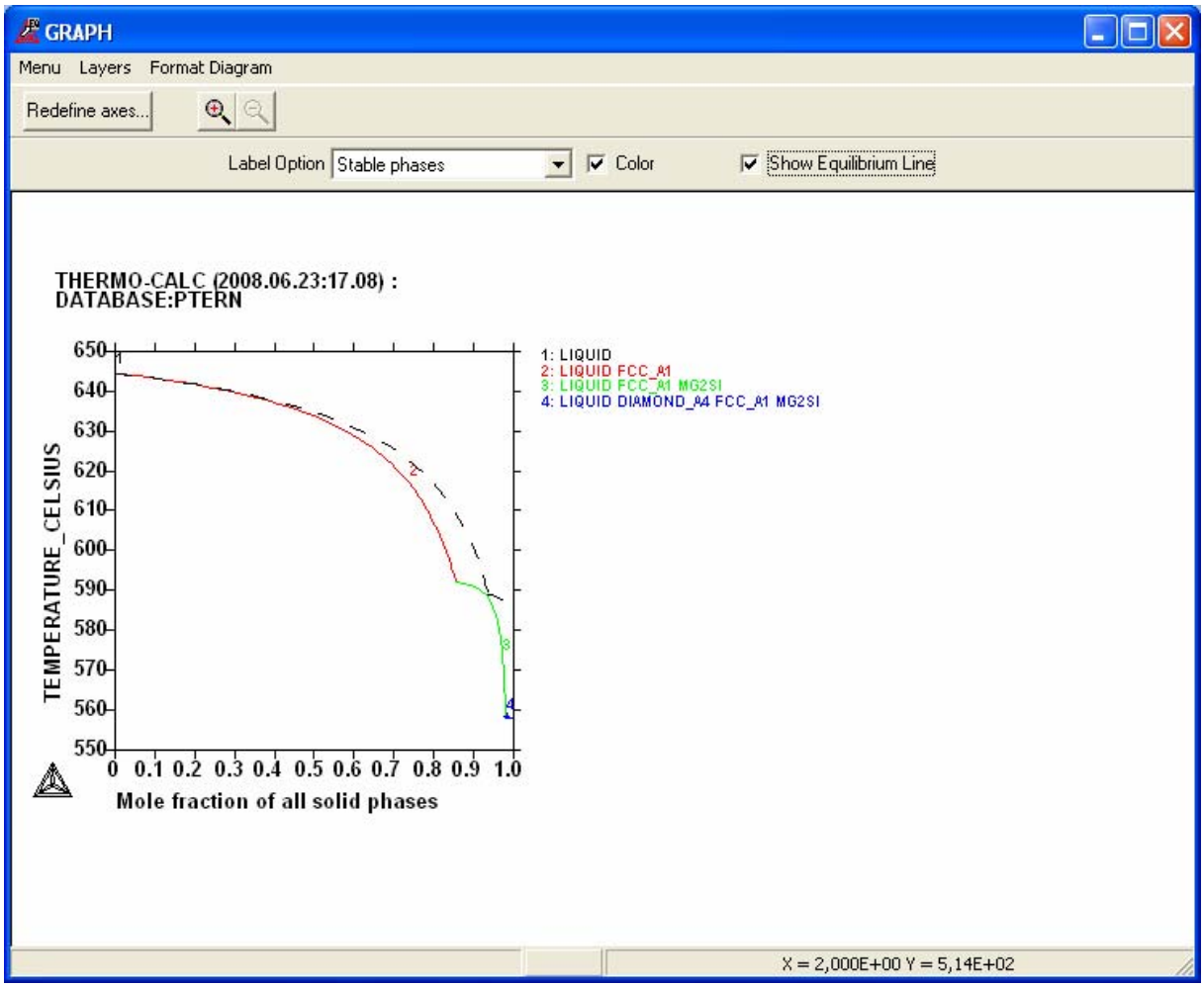
Select *PTERN* from the *Database* list and then click alloy elements *Al*, *Mg*, and *Si* in the periodic table. Click *Next*.

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

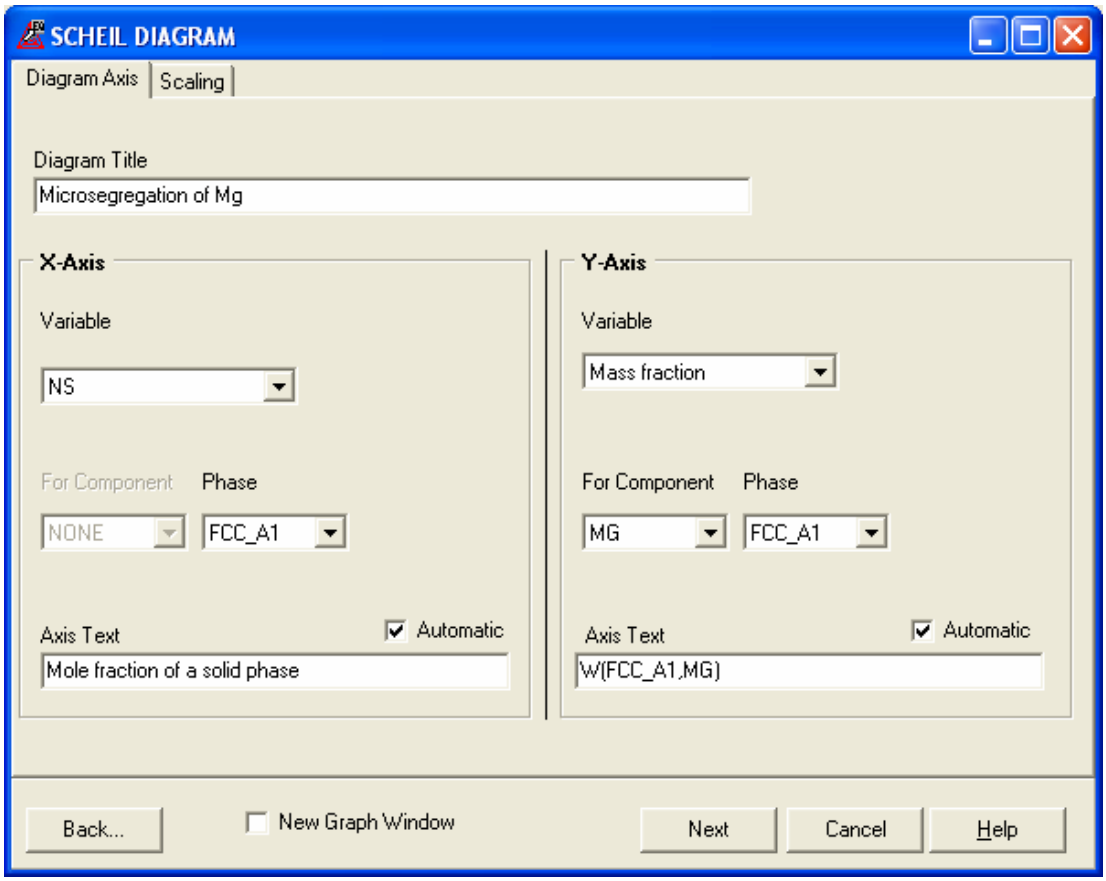


1. Accept the default X and Y –Axis variables by clicking *Next*. The solidification range diagram is plotted.

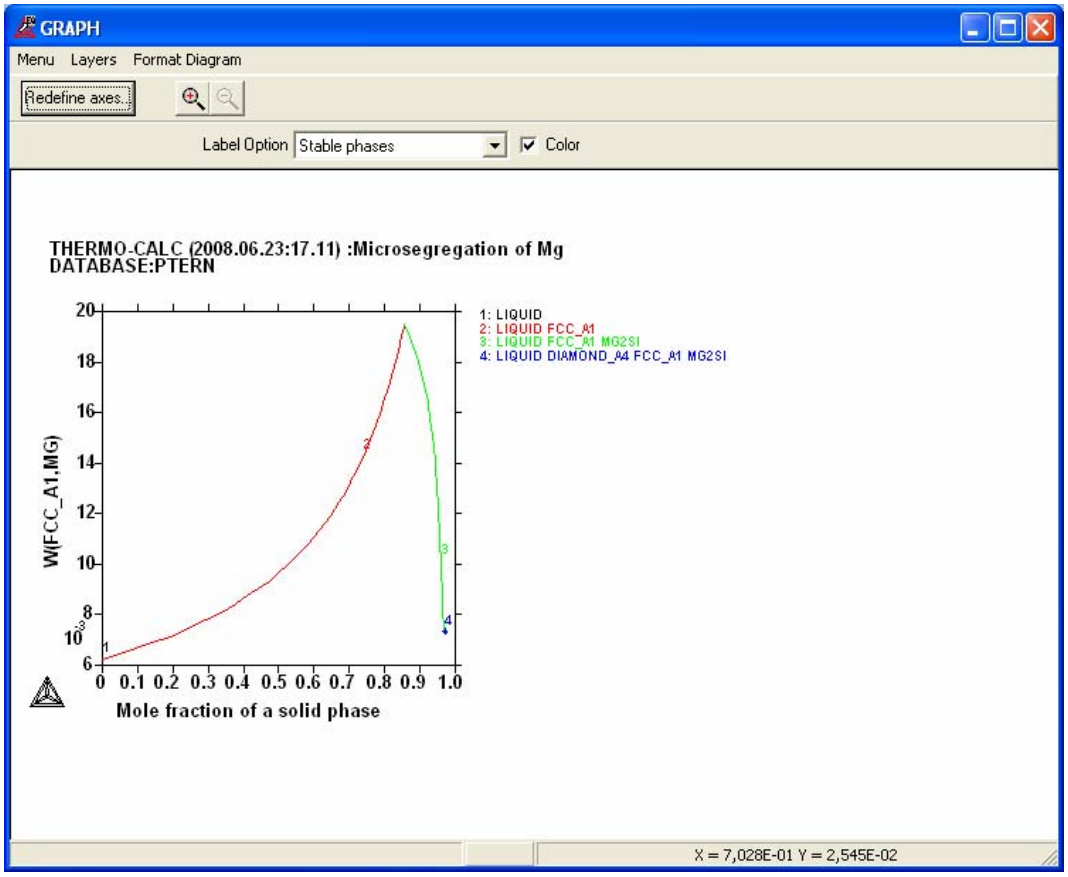
2. Check the *Show Equilibrium Line* box to add the equilibrium solidification curve.



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*



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

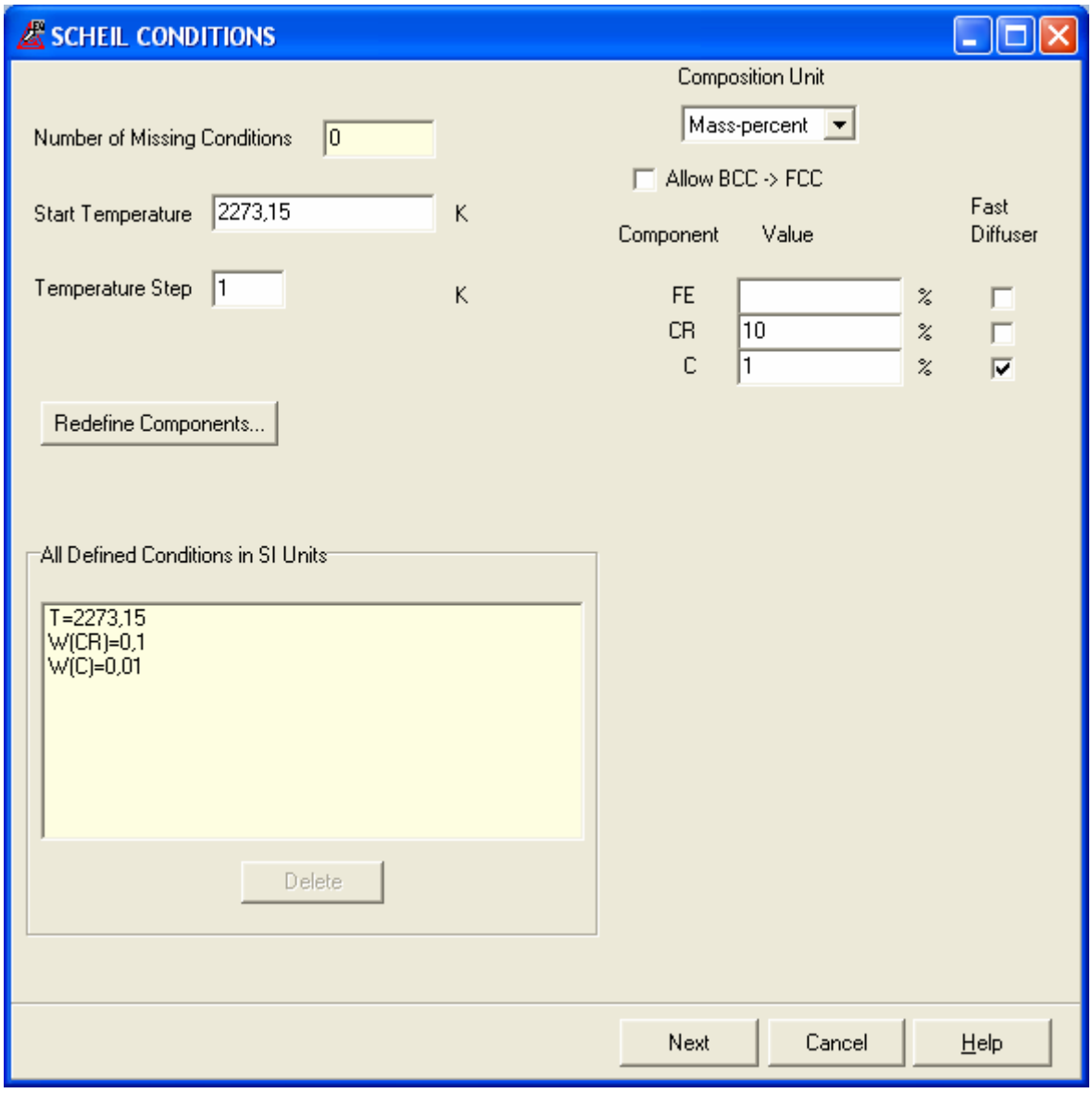


15 Scheil-Gulliver Simulation of Solidification for a Steel with Back Diffusion of Carbon in Solid Phases

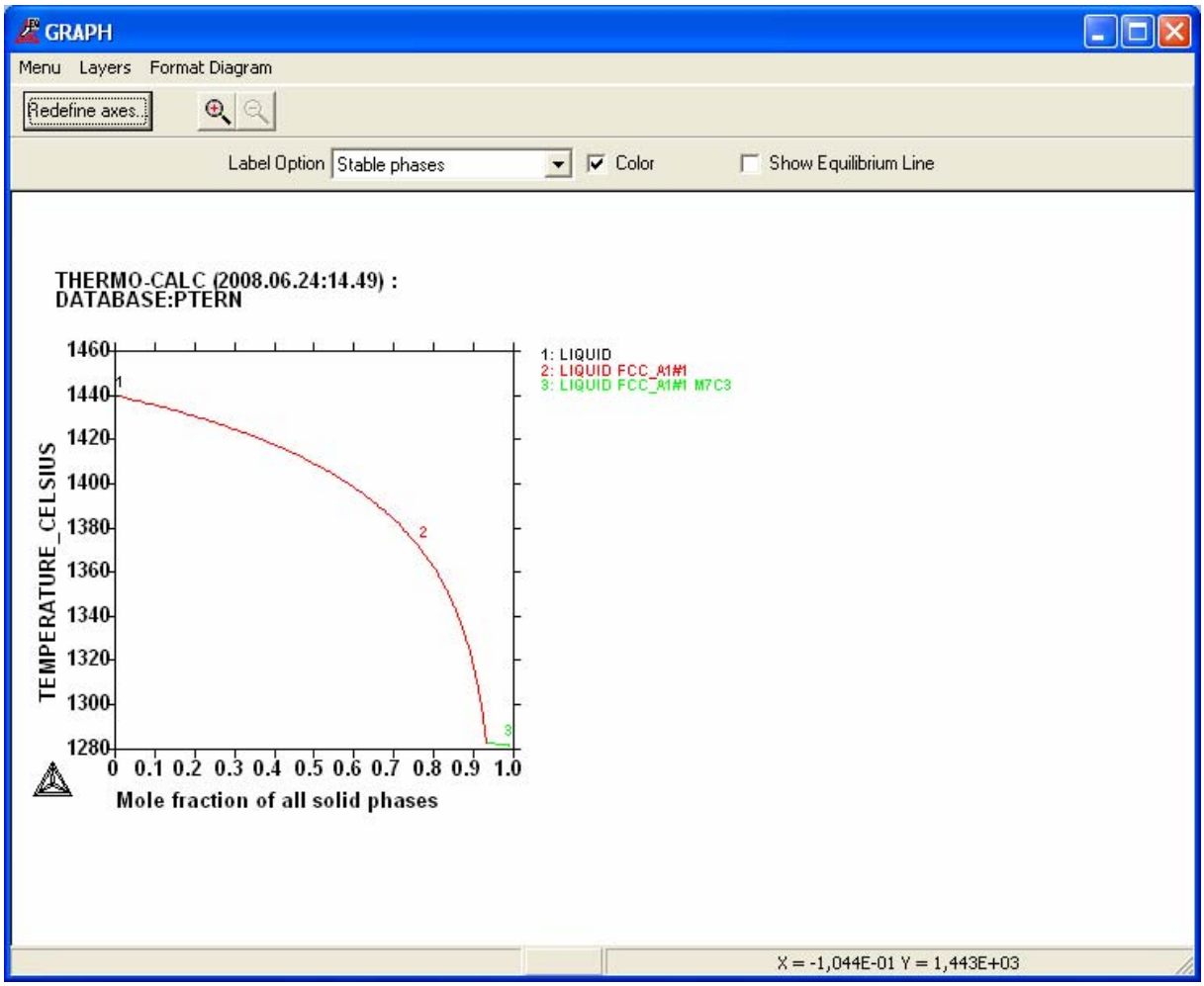
1. Click  in the MAIN window.

2. Select *PTERN* from the *Database* list and then click alloy elements *Fe*, *Cr*, and *C* in the periodic table. Click *Next*.

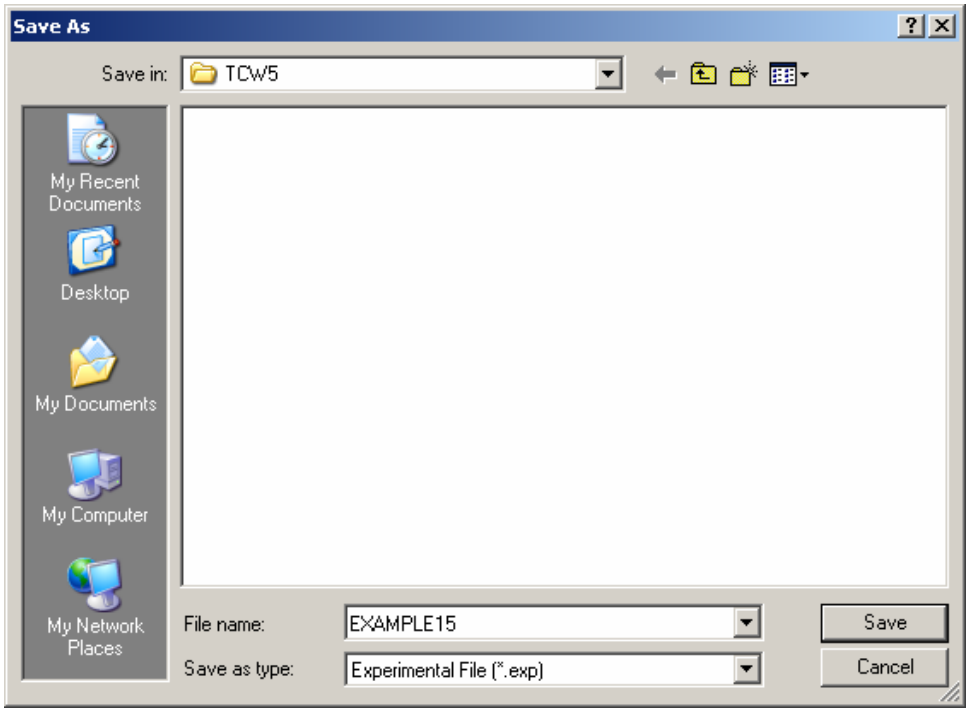
3. Specify the concentrations of C and Cr as *1* and *10 mass-percent*, respectively and check the *Fast Diffuser* box after C. Click *Next*.



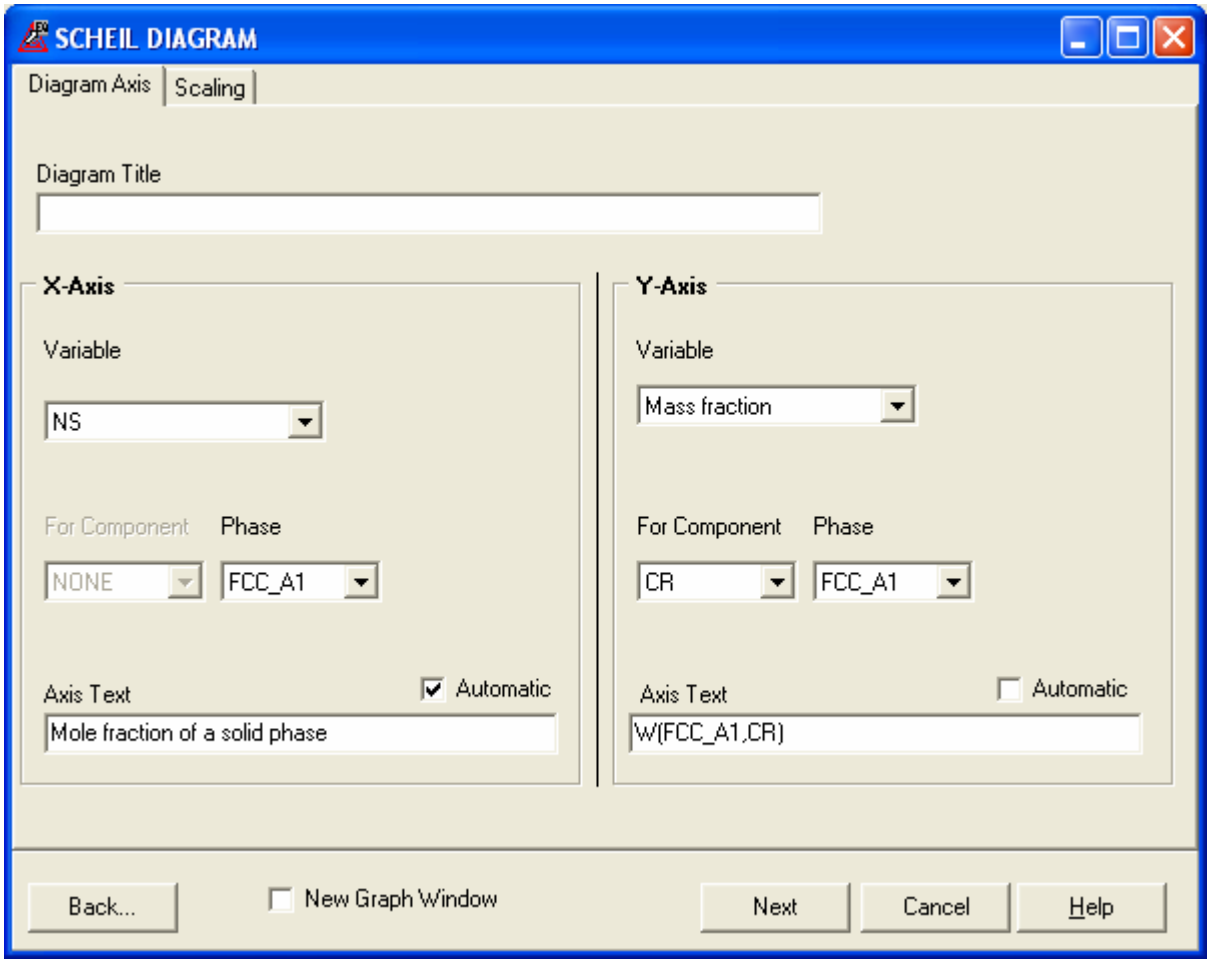
4. Accept the default X and Y -Axis variables by clicking *Next*. The solidification range diagram is plotted.



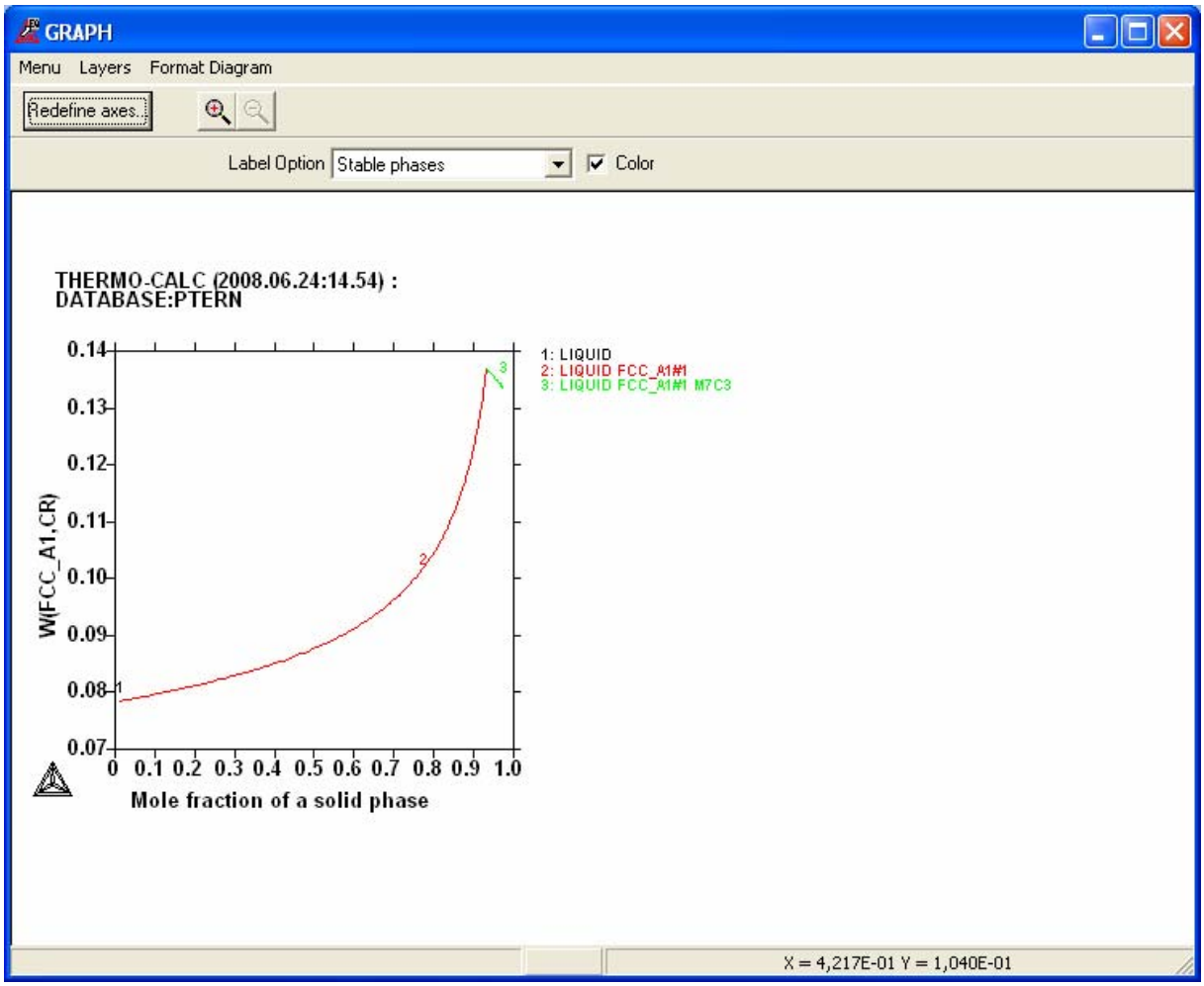
5. Click *Menu* → *Save*. Specify file type as Experimental File (*.exp) and file name as EXAMPLE15. Click *Save*.



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.*



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.

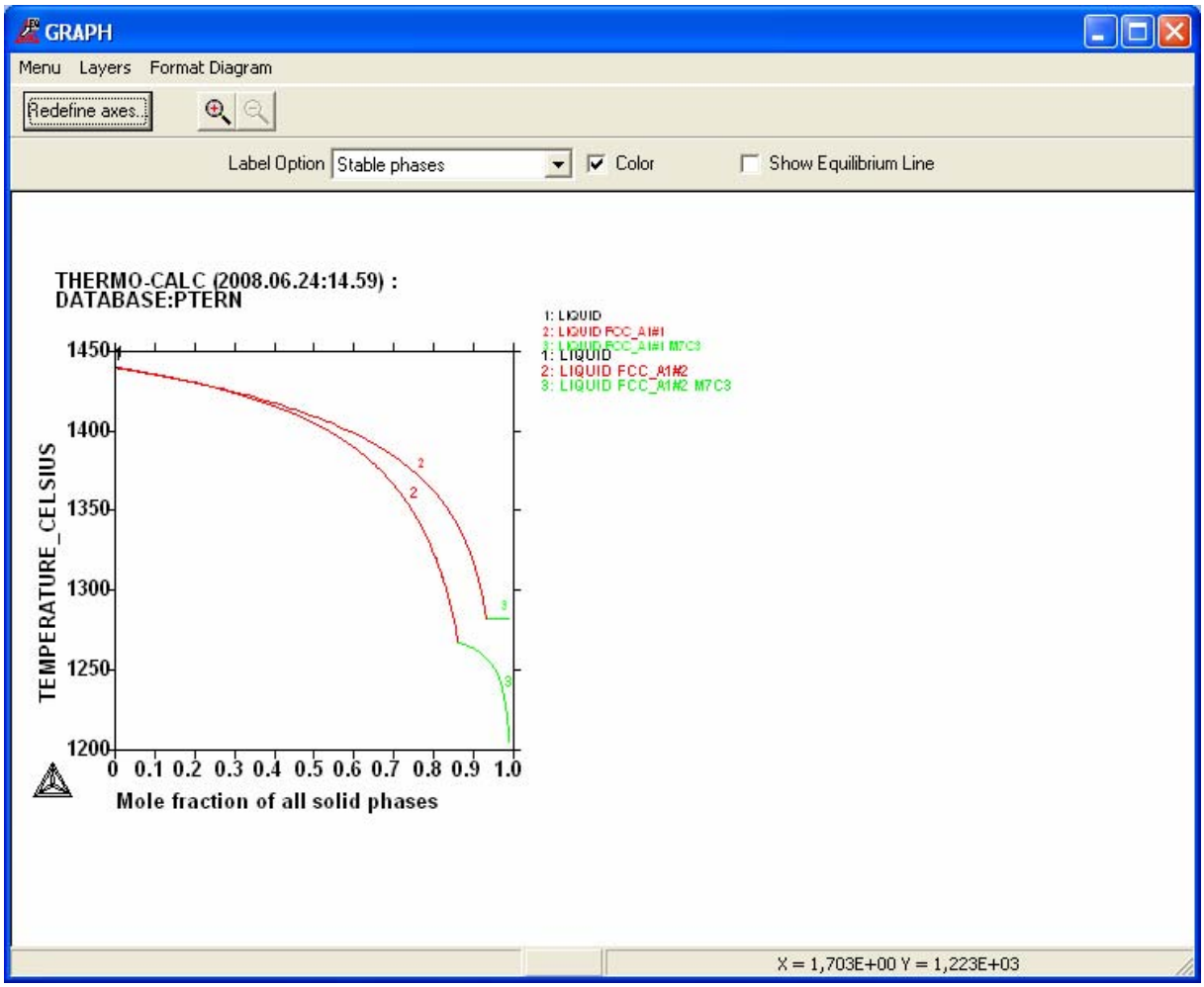
10. Click *Next*. The previously selected database and elements has been kept and no need to change.

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.

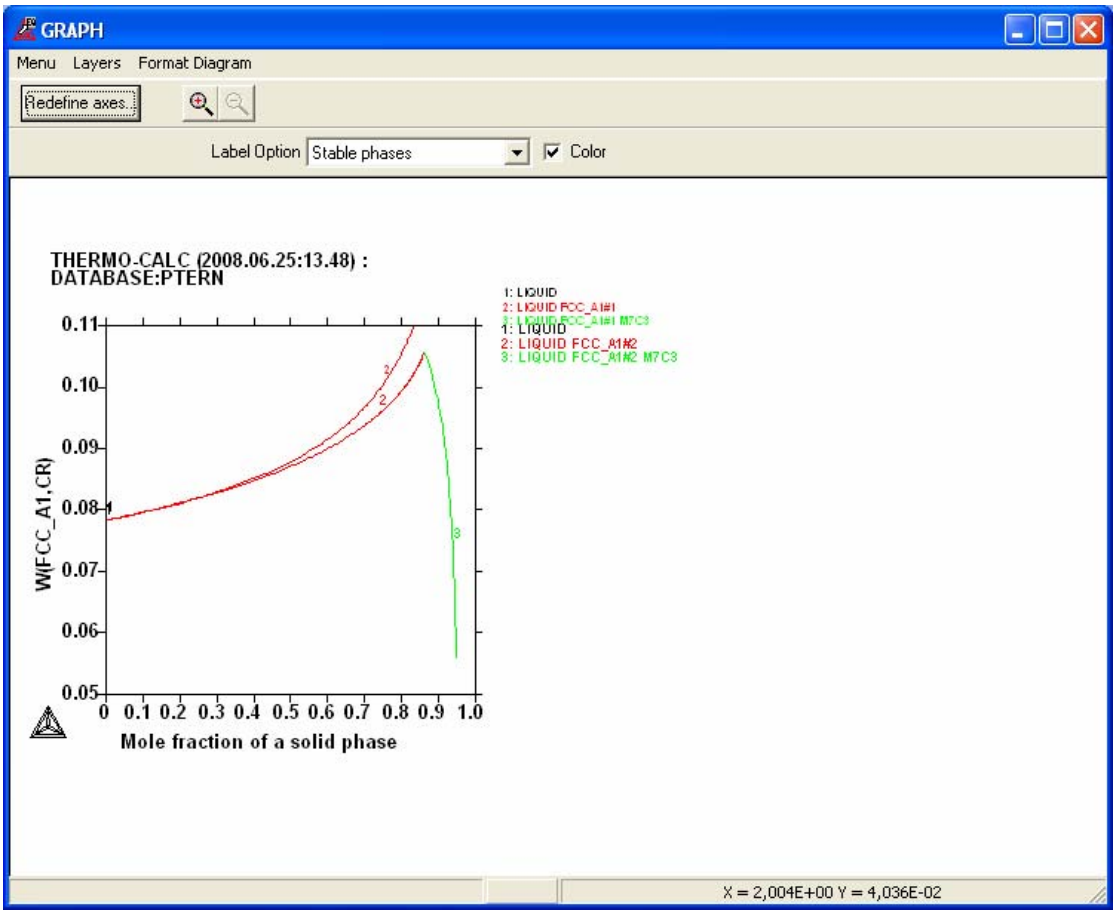
13. Click *Menu* → *Append* and then *Add*. Select file *EXAMPLE15.exp* and click *Open* followed by *OK (make sure the file has the box checked)*.

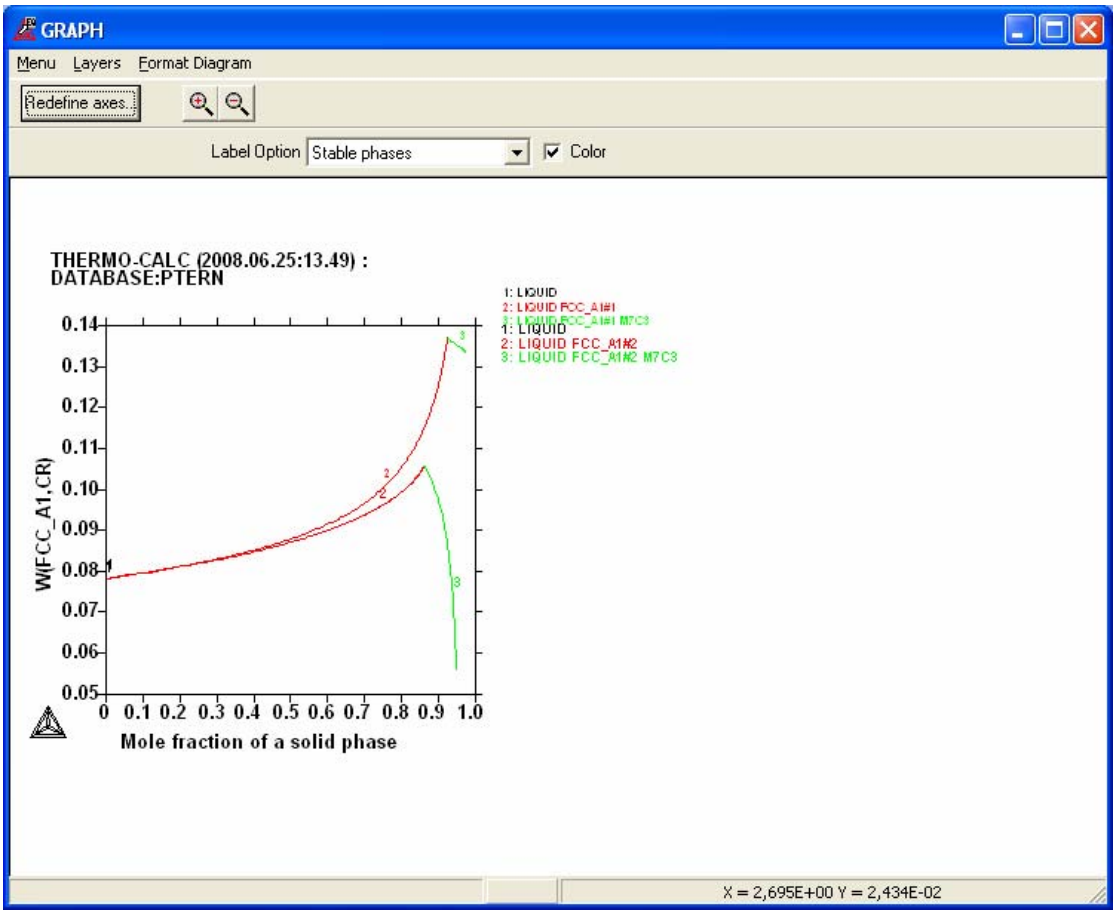
14. The solidification curve from the modified Scheil simulation is now superimposed on the result of the simple Scheil simulation.



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.

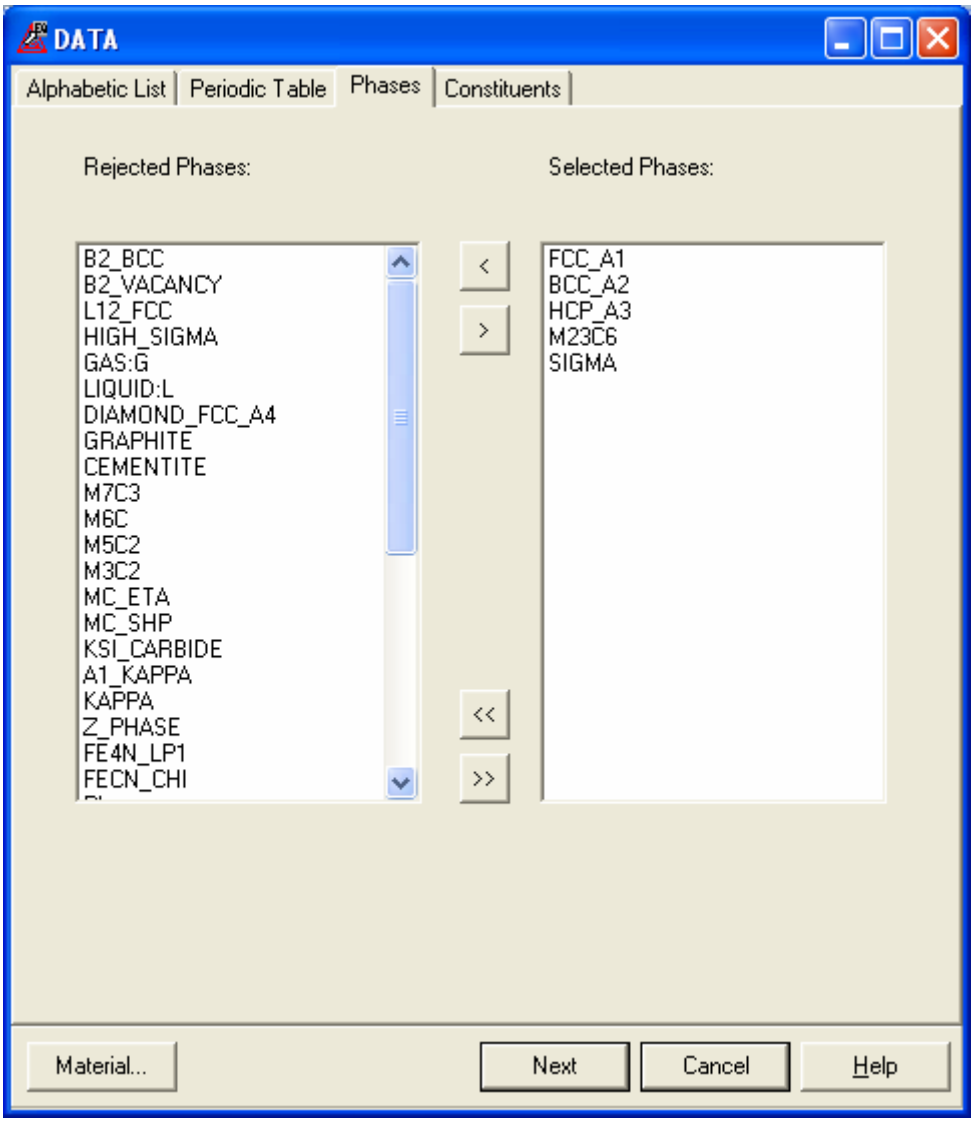

GRAPH
Menu Layers Format Diagram
Redefine axes.
Label Option Stable phases
Color
THERMO-CALC (2008.06.25:13.48) :
DATABASE:PTERN
1: LIQUID
2: LIQUID FCC_A1#1
3: LIQUID FCC_A1#2 M7C3
W(FCC_A1,CR)
0.11
0.10
0.09
0.08
0.07
0.06
0.05
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
Mole fraction of a solid phase
X = 2,004E+00 Y = 4,036E-02


GRAPH
Menu Layers Format Diagram
Redefine axes.
Label Option Stable phases
Color
THERMO-CALC (2008.06.25:13.49) :
DATABASE:PTERN
1: LIQUID
2: LIQUID FCC_A1#1
3: LIQUID FCC_A1#2 M7C3
W(FCC_A1,CR)
0.14
0.13
0.12
0.11
0.10
0.09
0.08
0.07
0.06
0.05
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
Mole fraction of a solid phase
X = 2,695E+00 Y = 2,434E-02

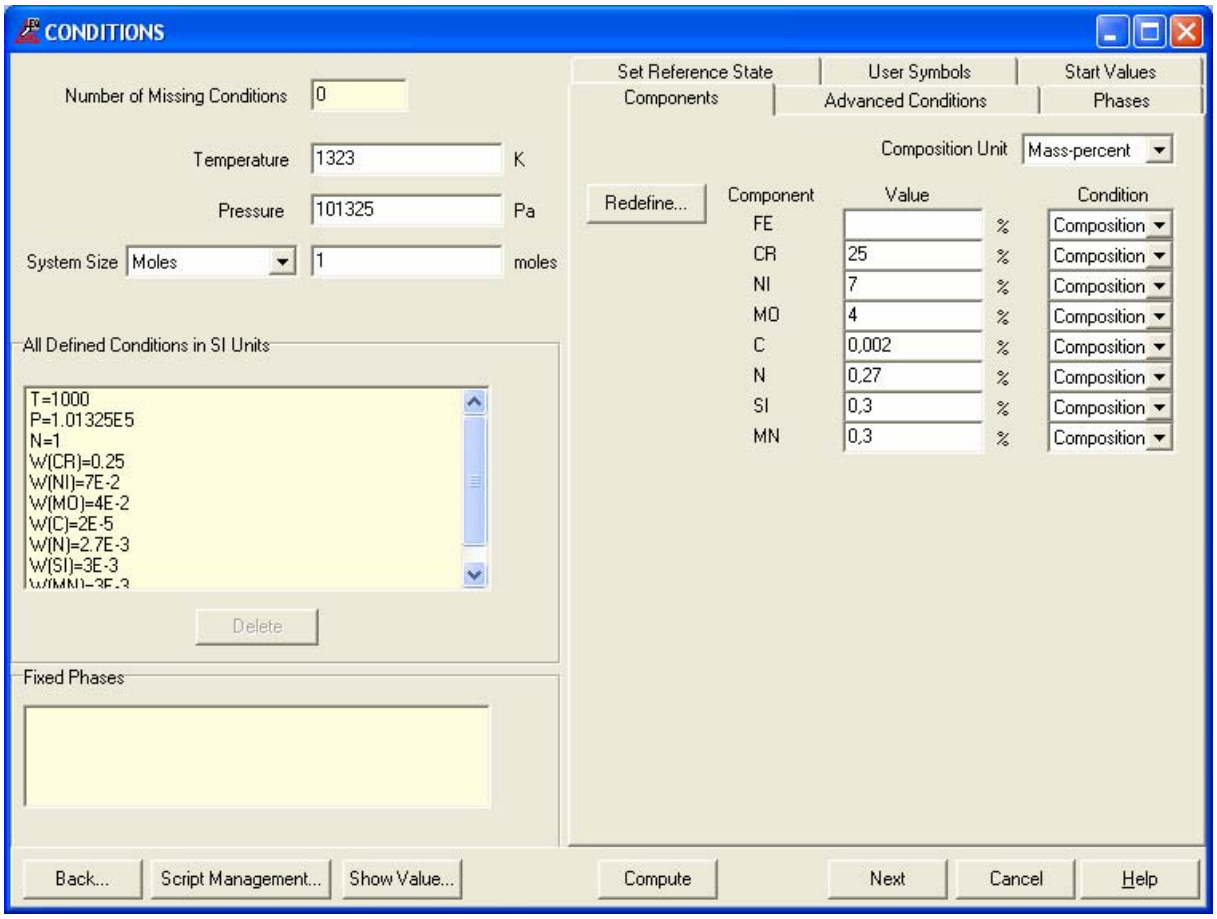
16 Calculation of Pitting Resistance Equivalence (PRE) for a Duplex Stainless Steel

1. Click *Elements* in the MAIN window.

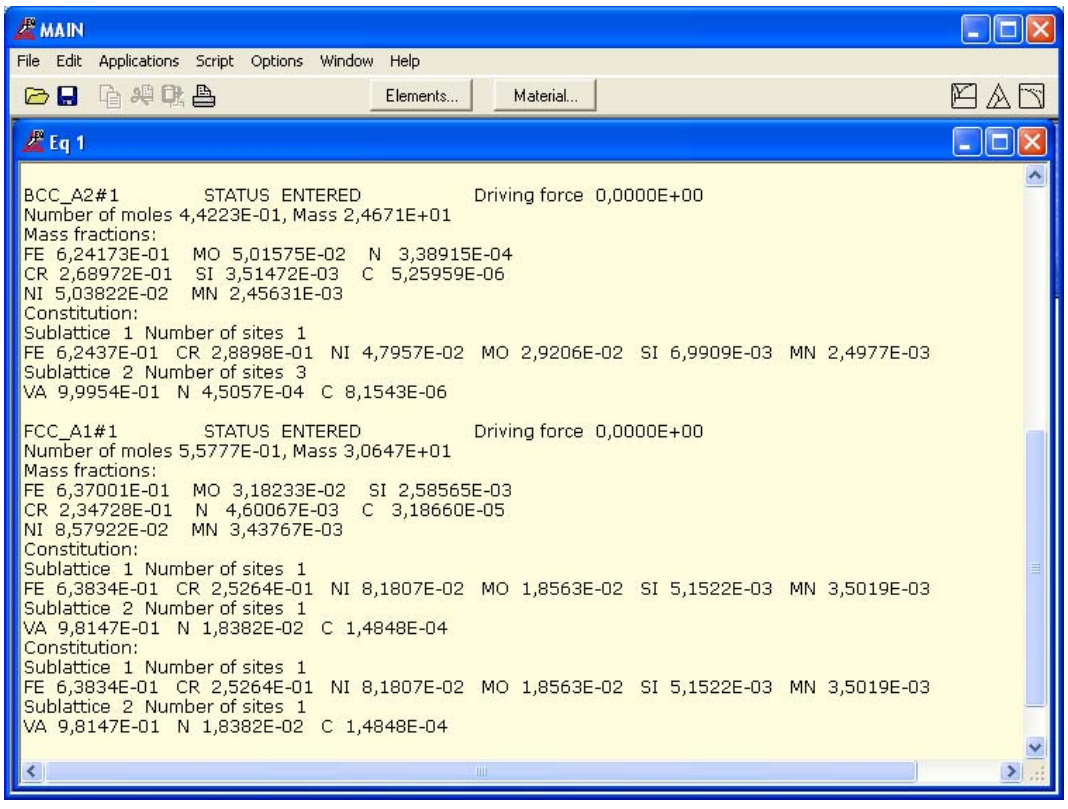
2. Select *TCFE6* under the Database option and then click alloy elements *Fe*, *Cr*, *Ni*, *Mo*, *C*, *N*, *Si*, and *Mn* in the periodic table. Select the *Phases* tab. Click << to reject all phases first, and then mark the phases *FCC_A1*, *BCC_A2*, *HCP_A3*, *M23C6*, and *SIGMA* and click > to restore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



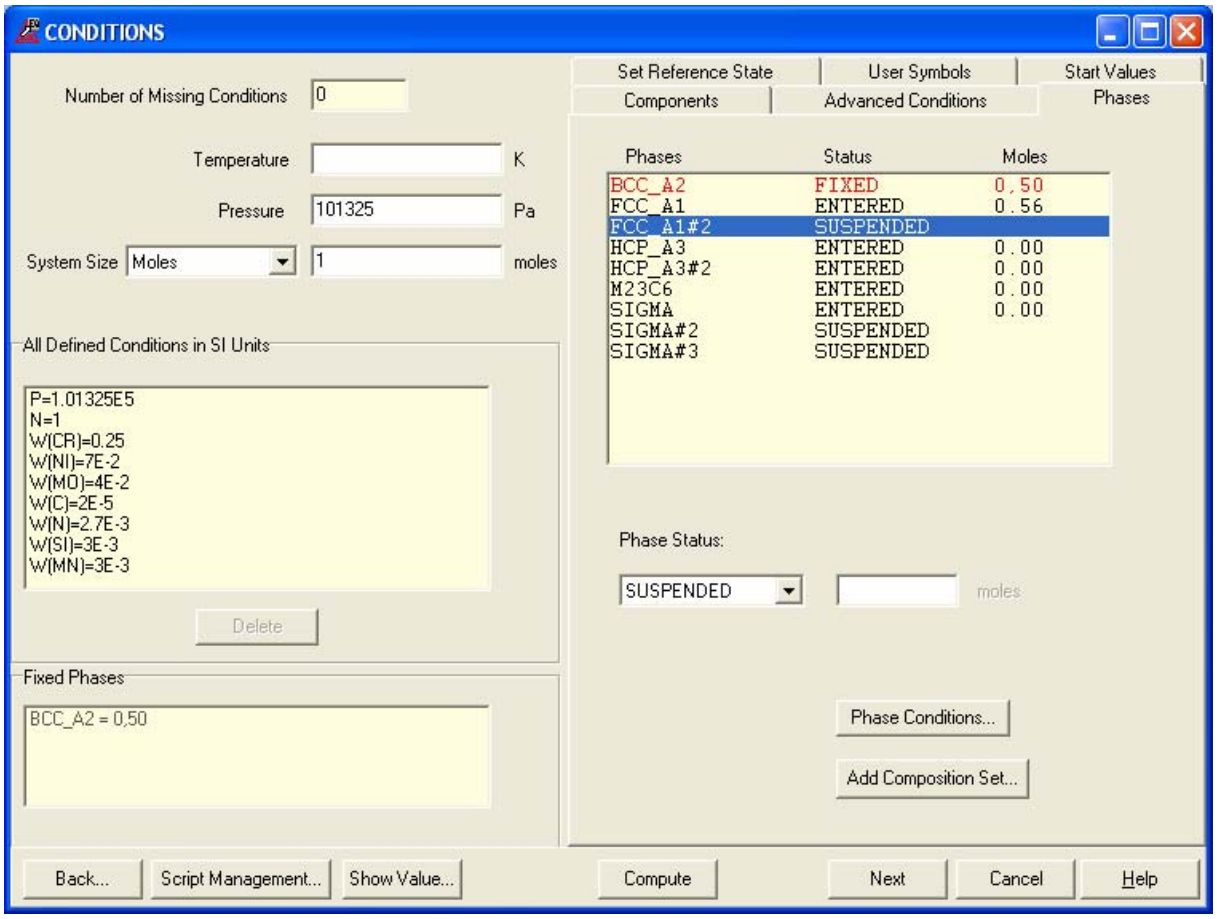
3. Click *Next*. Specify the concentrations of CR, NI, MO, C, N, SI, and MN as *25*, *7*, *4*, *0.002*, *0.27*, *0.3*, and *0.3*, mass-percent respectively. Set start temperature to *1323 K*. The default temperature unit can be changed by selecting *Output* in the *Options* menu in the MAIN window.



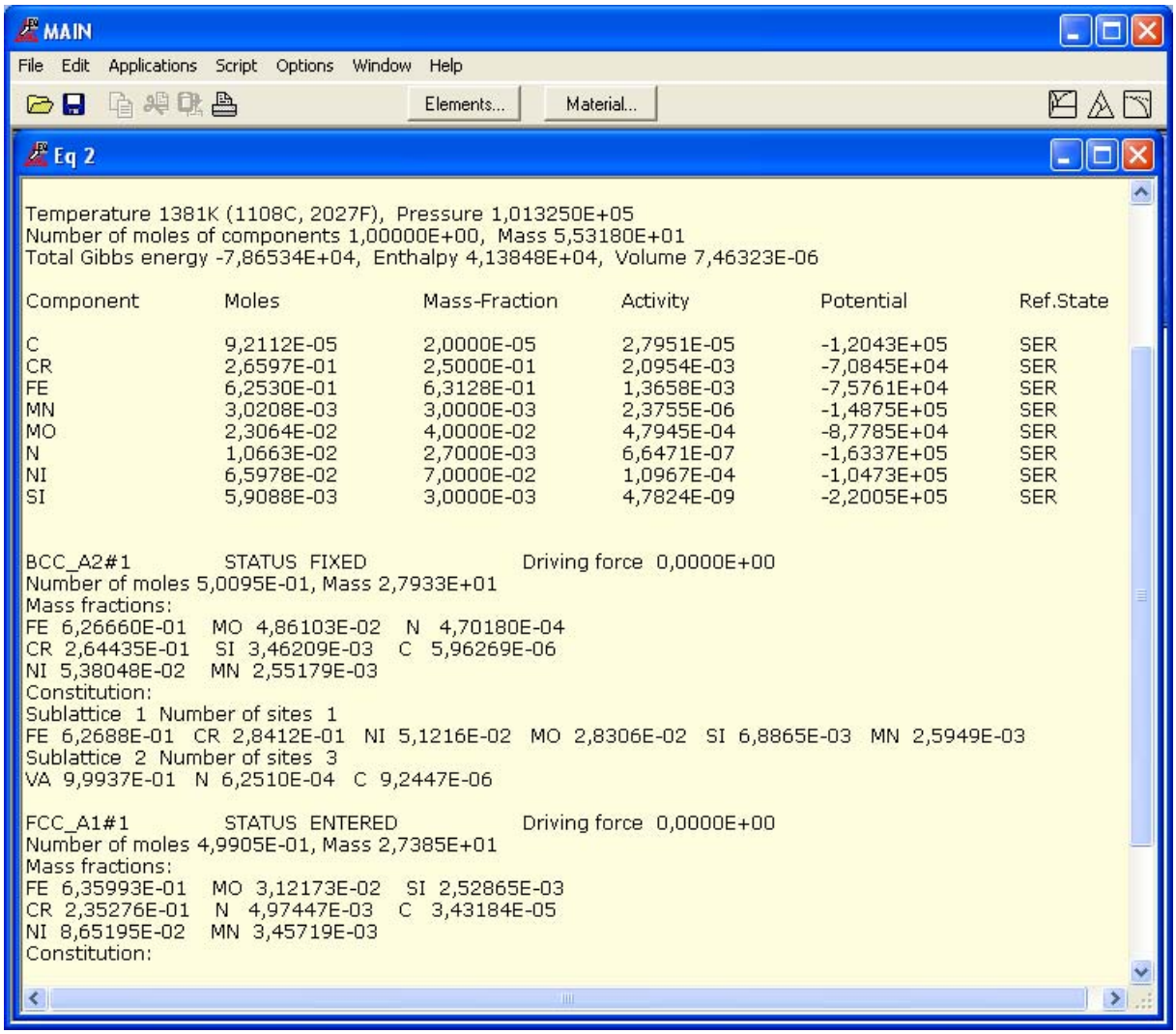
4. Click *Compute*. The phase equilibrium is calculated and the result is shown in a text window.



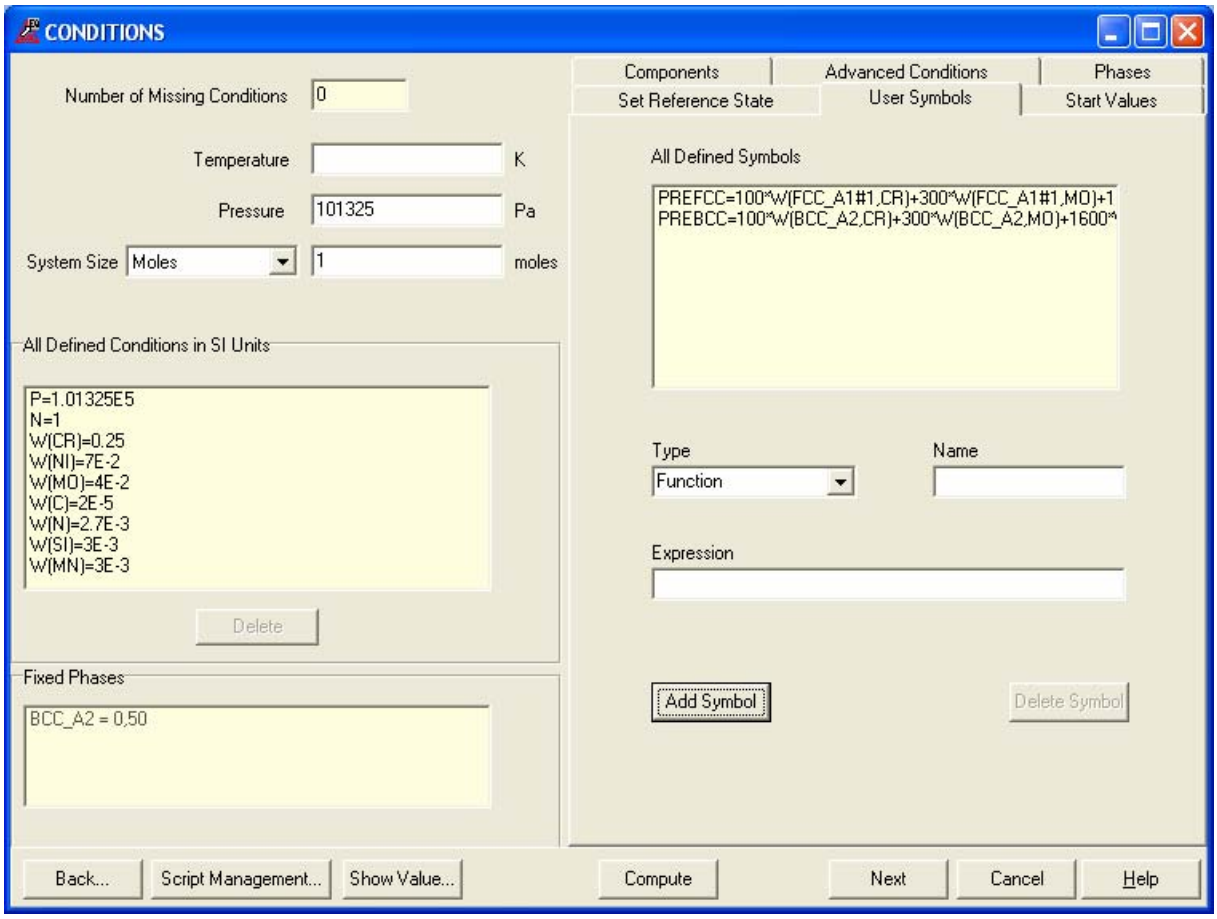
5. Select the *Phases* tab on the CONDITIONS window. Choose *BCC_A2* and change the *Phase Status* option to *FIXED* with an amount of *0.5* moles. In a similar way, change the phase status of *FCC_A1#2* to *SUSPENDED* in order to avoid possible trouble with this suppose-to-be MC carbide phase during 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*.



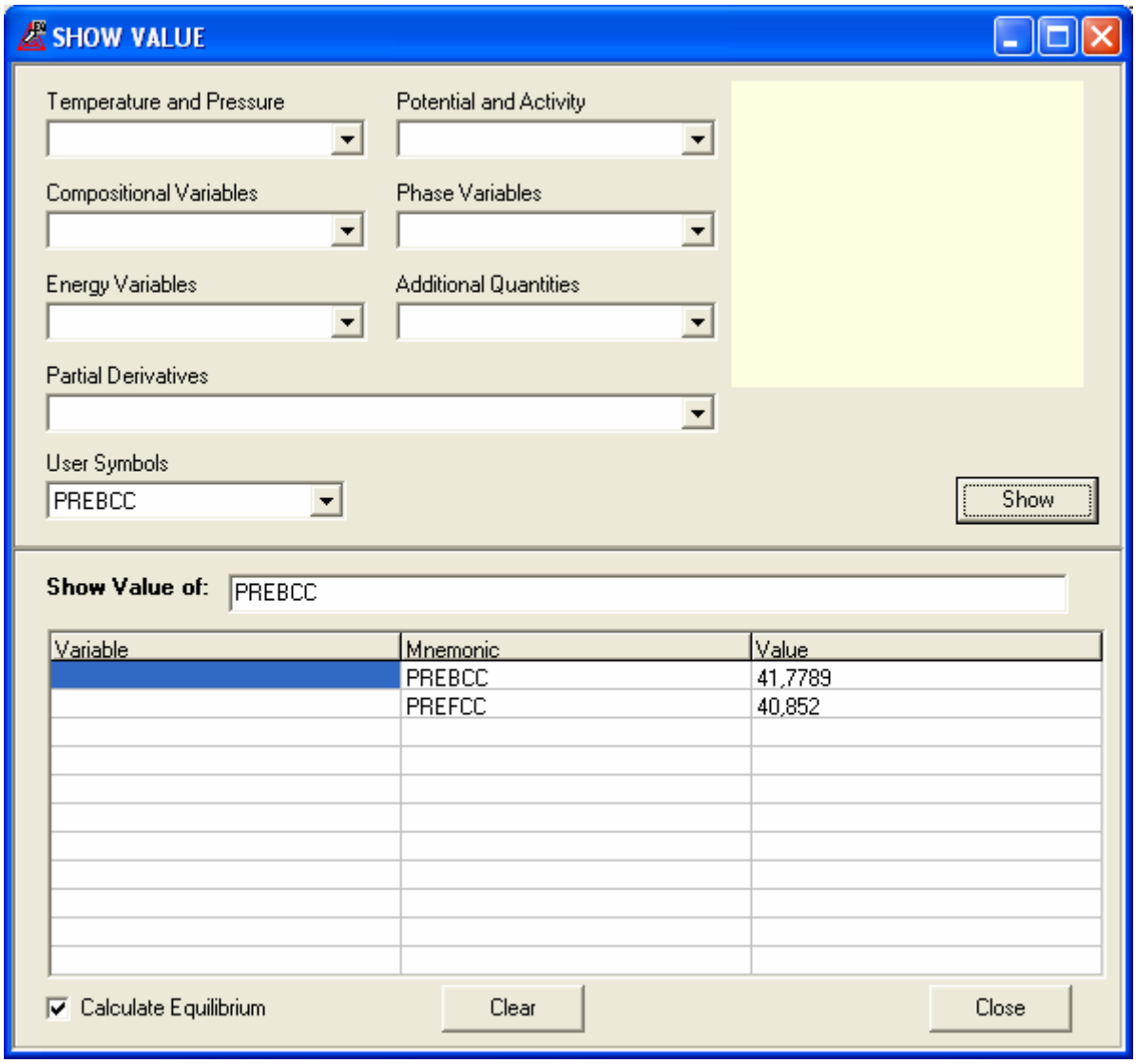
6. Click *Compute*. The equilibrium under the defined conditions is calculated. The temperature for developing the duplex structure in this steel is obtained and can be found in the equilibrium result window.



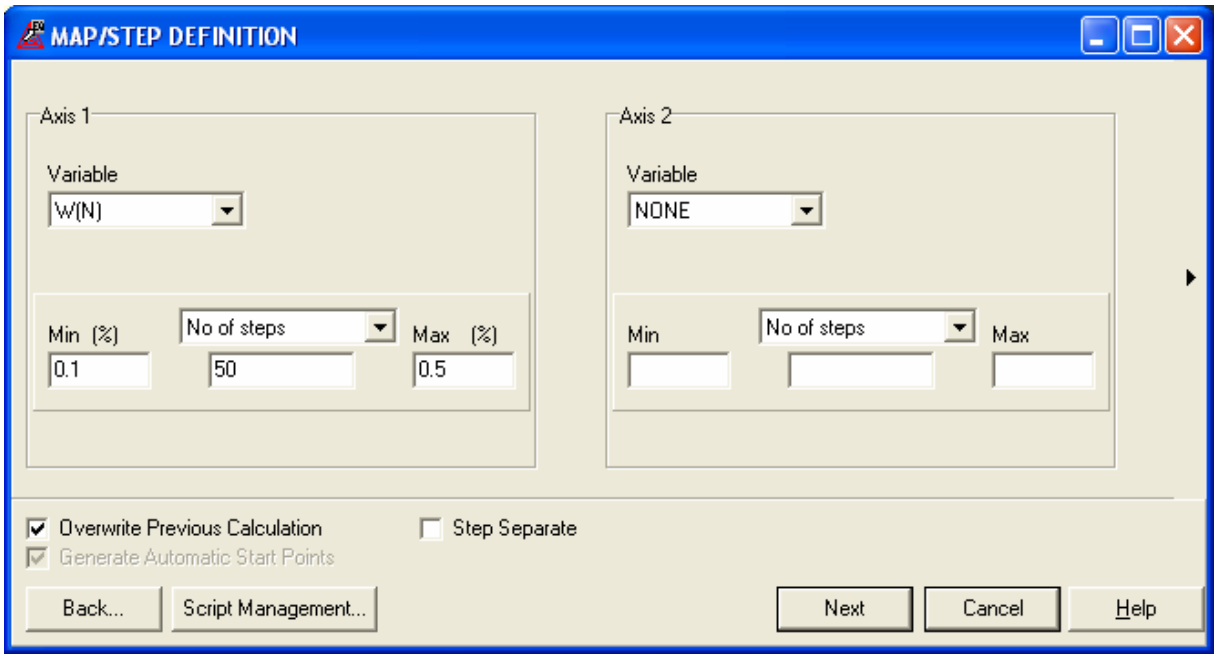
7. Go back to the CONDITIONS window and select the *User Symbols* tab to define two PRE functions. In the *Name* box, input *PREFCC*. In the *Expression* box, input *100*W(FCC,CR)+300*W(FCC,MO)+1600*W(FCC,N)***.** Click *Add Symbol*. Then, in a similar way, enter the PRE function for BCC_A2, i.e., enter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



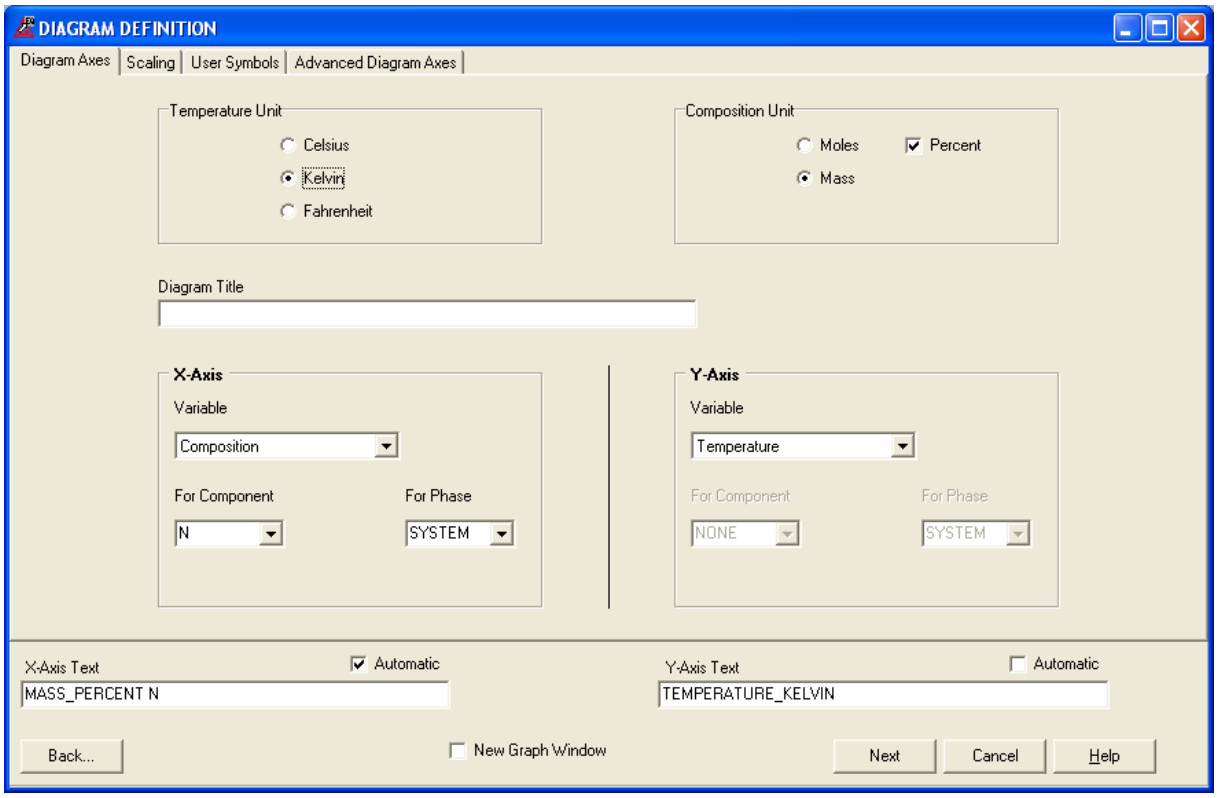
8. Let's have a look of the PRE values now. Click *Show Value*. A window pops up. Choose the function *PREFCC* from the *User Symbols* list and click *Show*. Do same with PREBCC. Close the window by clicking *Close*.



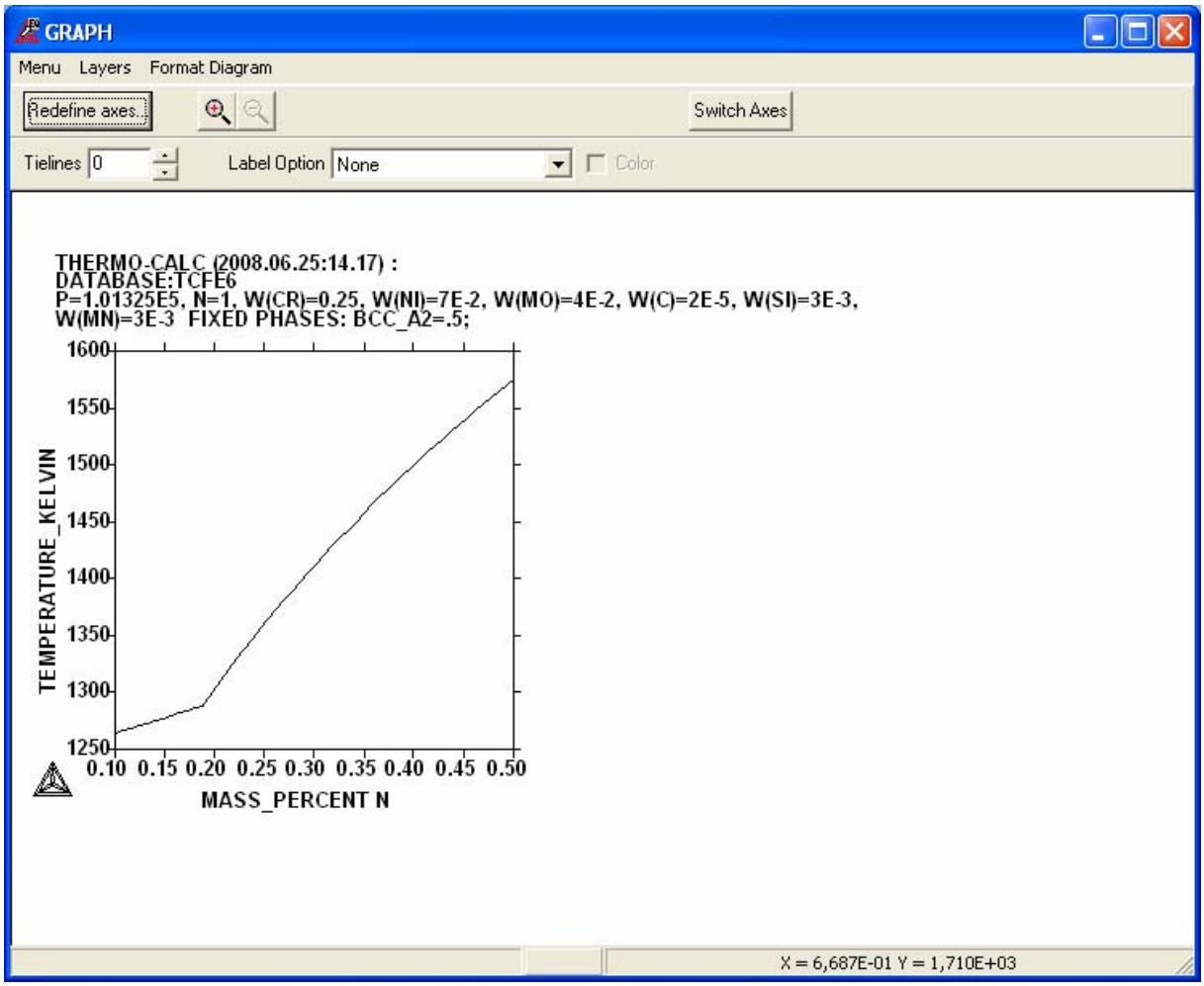
9. Calculate the PRE of duplex steel with different content of nitrogen. Click *Next* on the CONDITIONS window. The MAP/STEP DEFINITION window appears. Select *W(N)* for *Axis 1* and change Min value to *0.1* and Max value to *0.5*. Click *Next*.



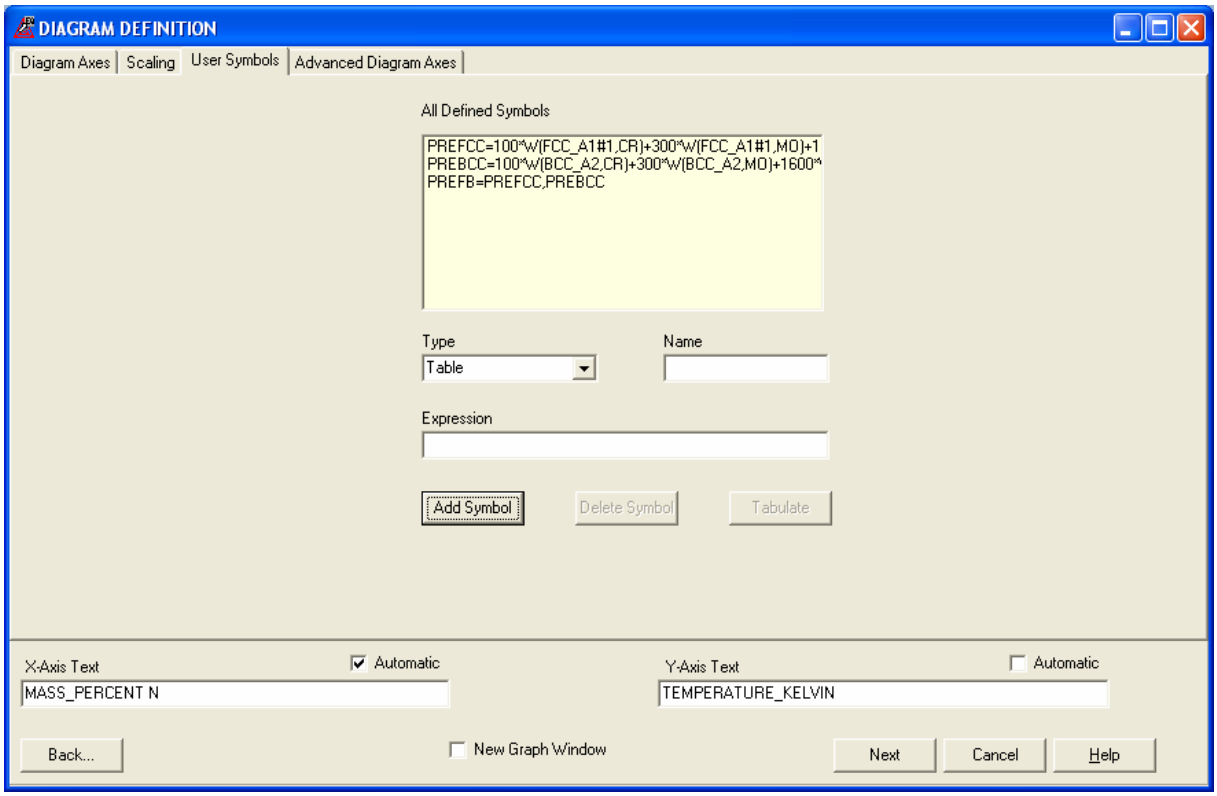
10. The DIAGRAM DEFINITION window appears. First let's see how the temperature for the formation of duplex structure varies with nitrogen content. Select *Mass Percent* for the X-Axis and *Temperature Kelvin* for the Y-Axis. Click *Next.*



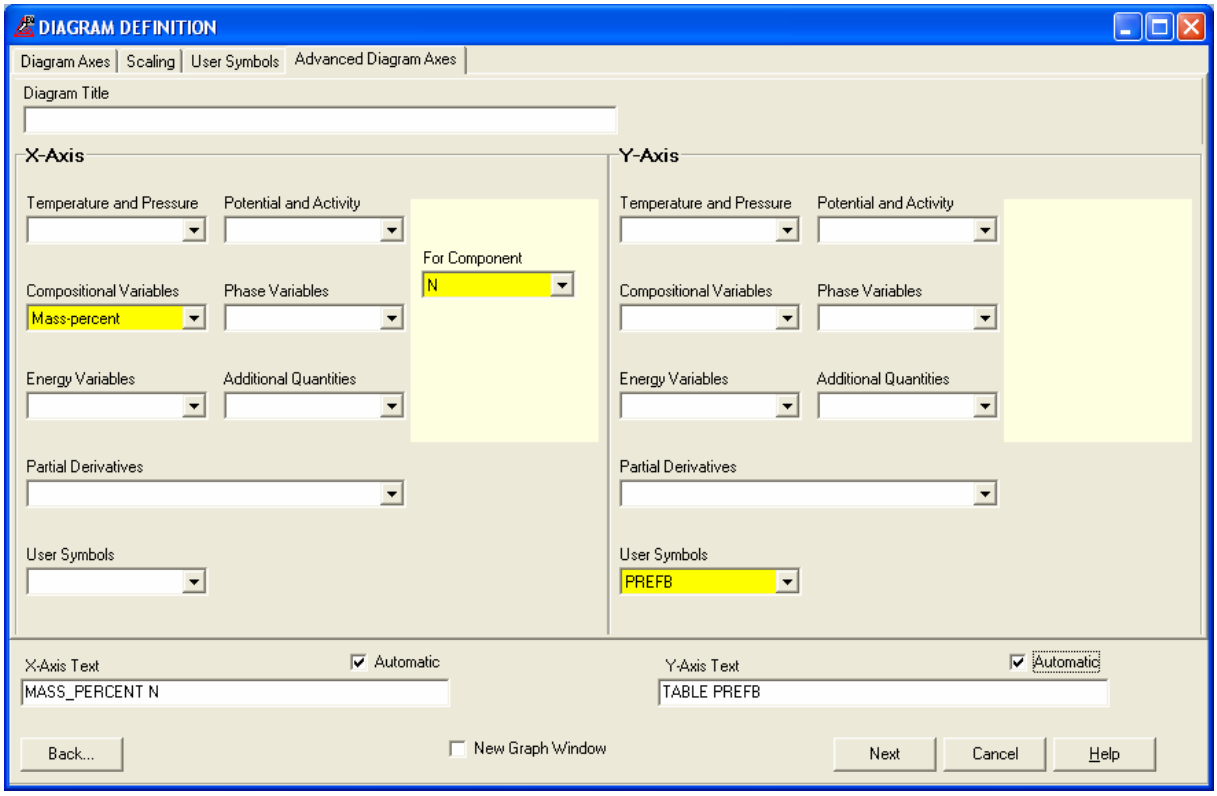
11. The dependence of temperature on nitrogen concentration is shown for the steel with duplex structure.



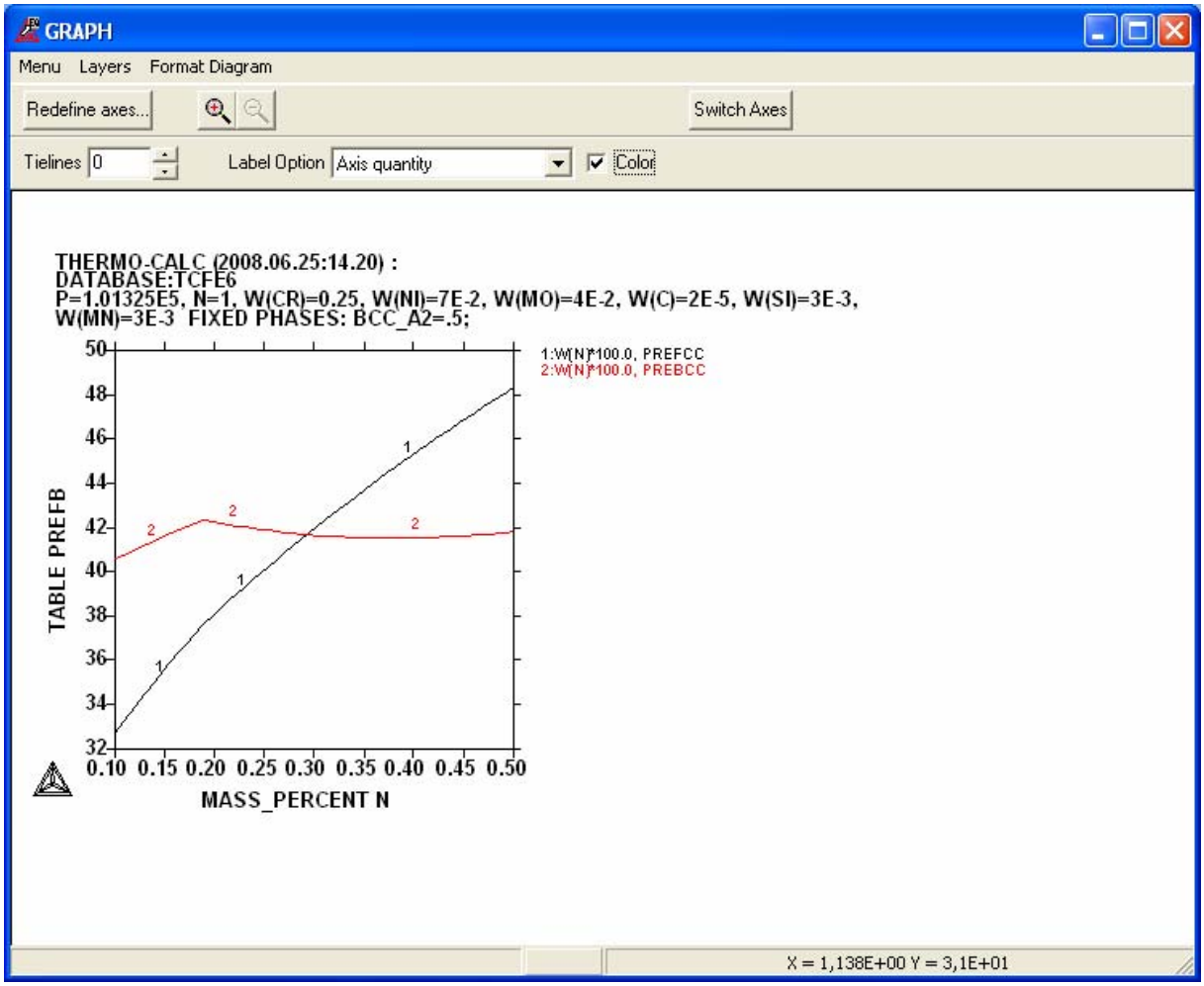
12. Click *Redefine*. Select the *User Symbols* tab. Change symbol *Type* to *Table*. Enter name *PREFB*. Enter expression *PREFCC*, *PREBCC*, click *Add Symbol*.



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



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

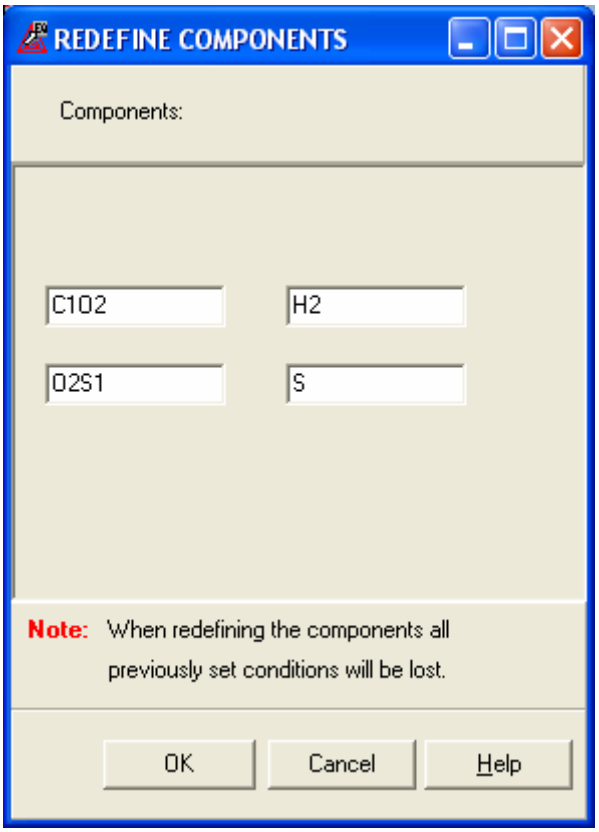


17 Calculation of Speciation of a Gas

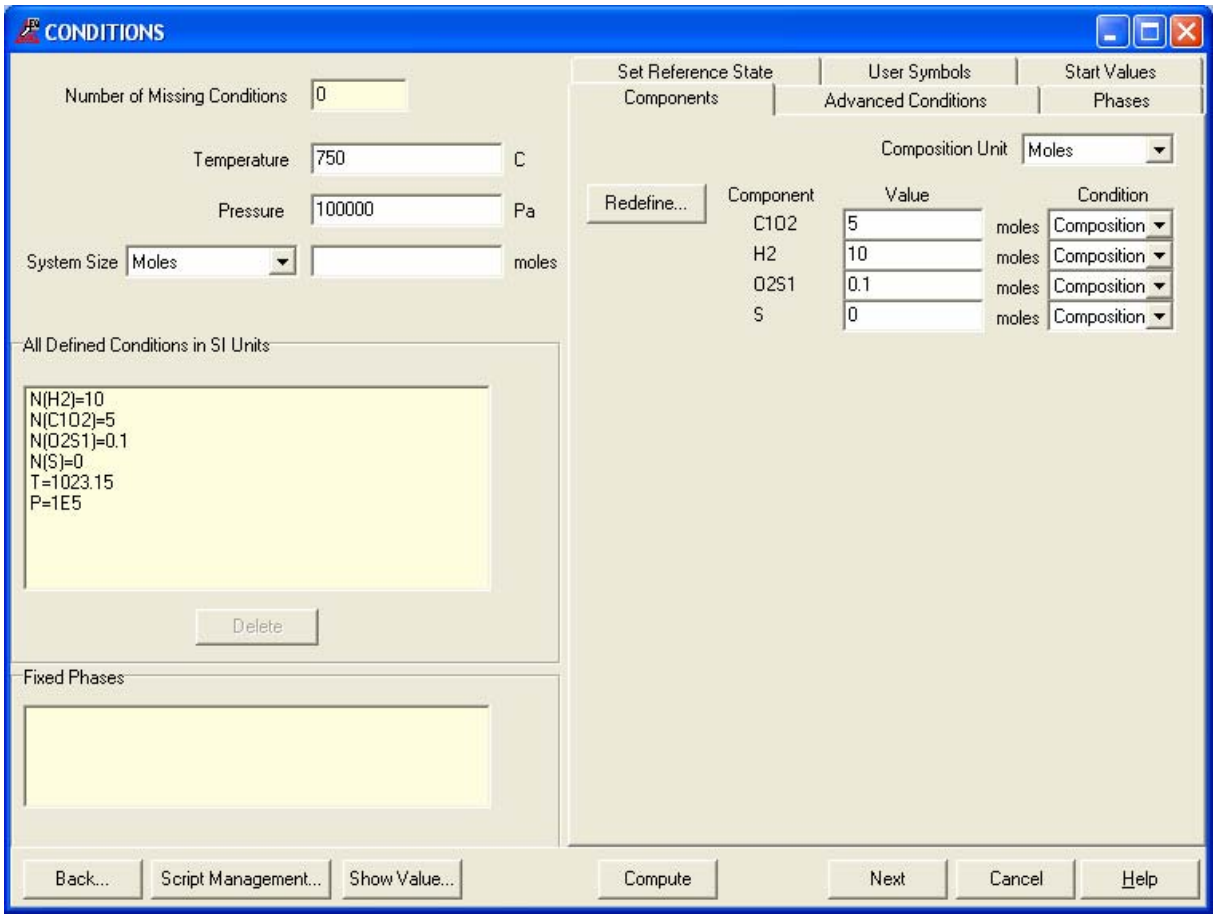
1. Click *Elements* in the MAIN window.

2. Select *SSUB4* from the Database list and then click elements *C*, *H*, *O*, and *S* in the periodic table. Click *Next*.

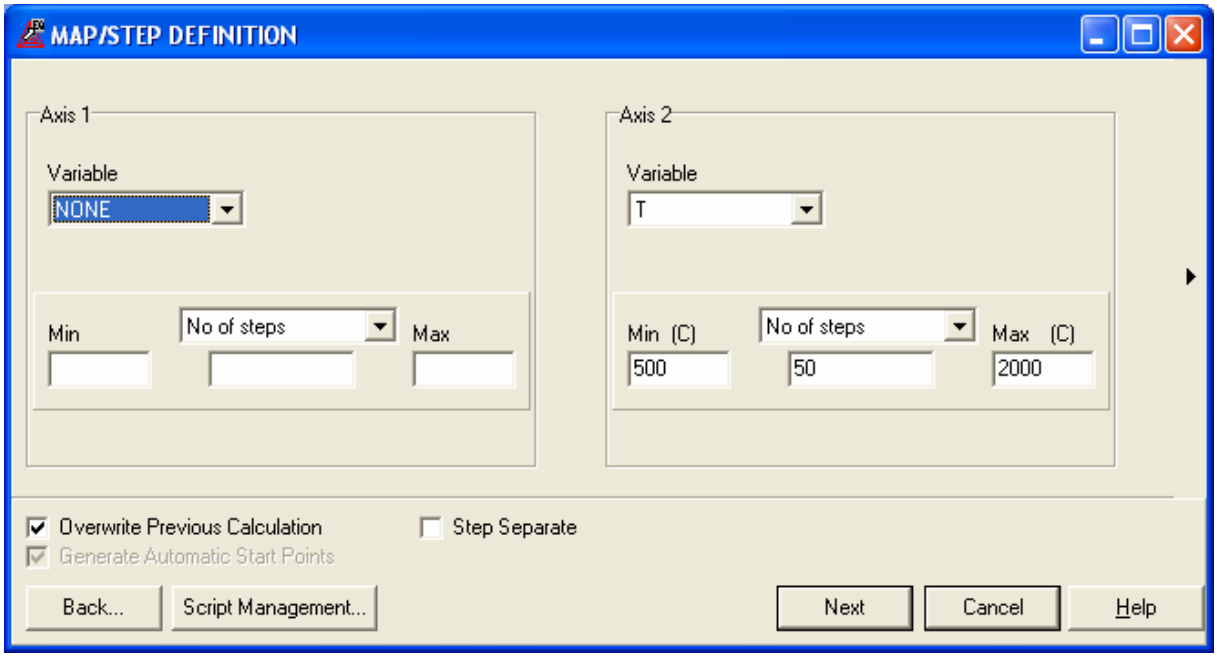
3. Click *Redefine*. In the REDEFINE COMPONENTS window, change C to *C1O2*, H to *H2*, O to *O2S1*. Click *OK*.



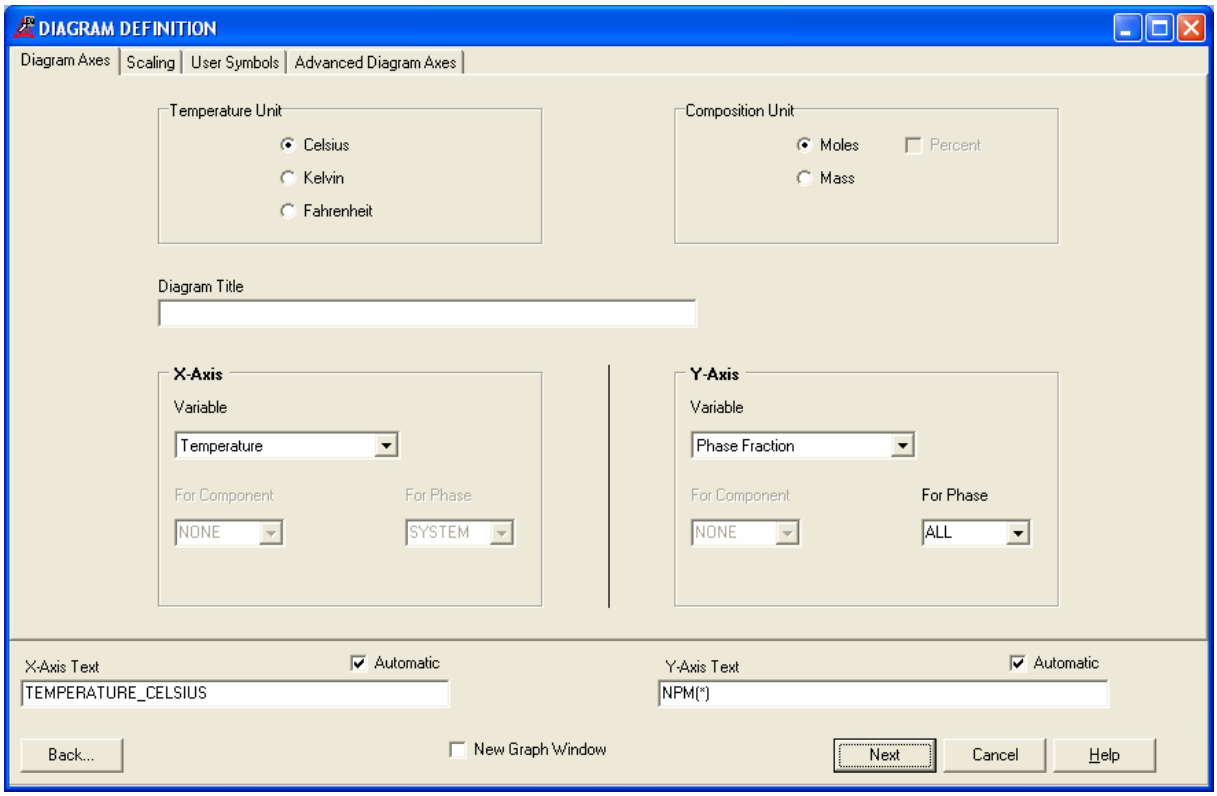
4. Select *Moles* as *Default Unit*. Enter value 5 for C1O2, *10* for H2, *0.1* for O2S1, and *0* for S. Set the temperature to *750* ºC and the pressure to *1E5*. Click *Next*.



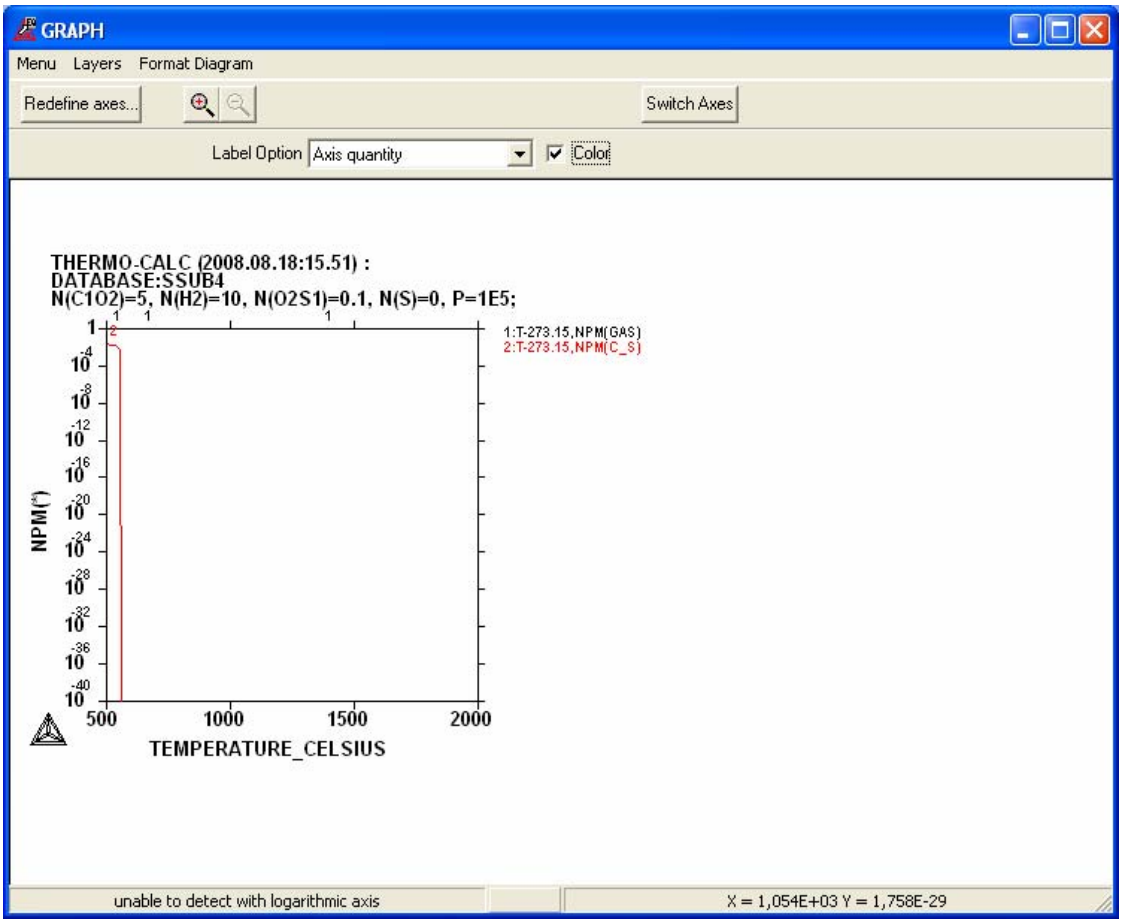
5. Keep the temperature variable for *Axis 2* and change the variable of *Axis 1* to *NONE*.



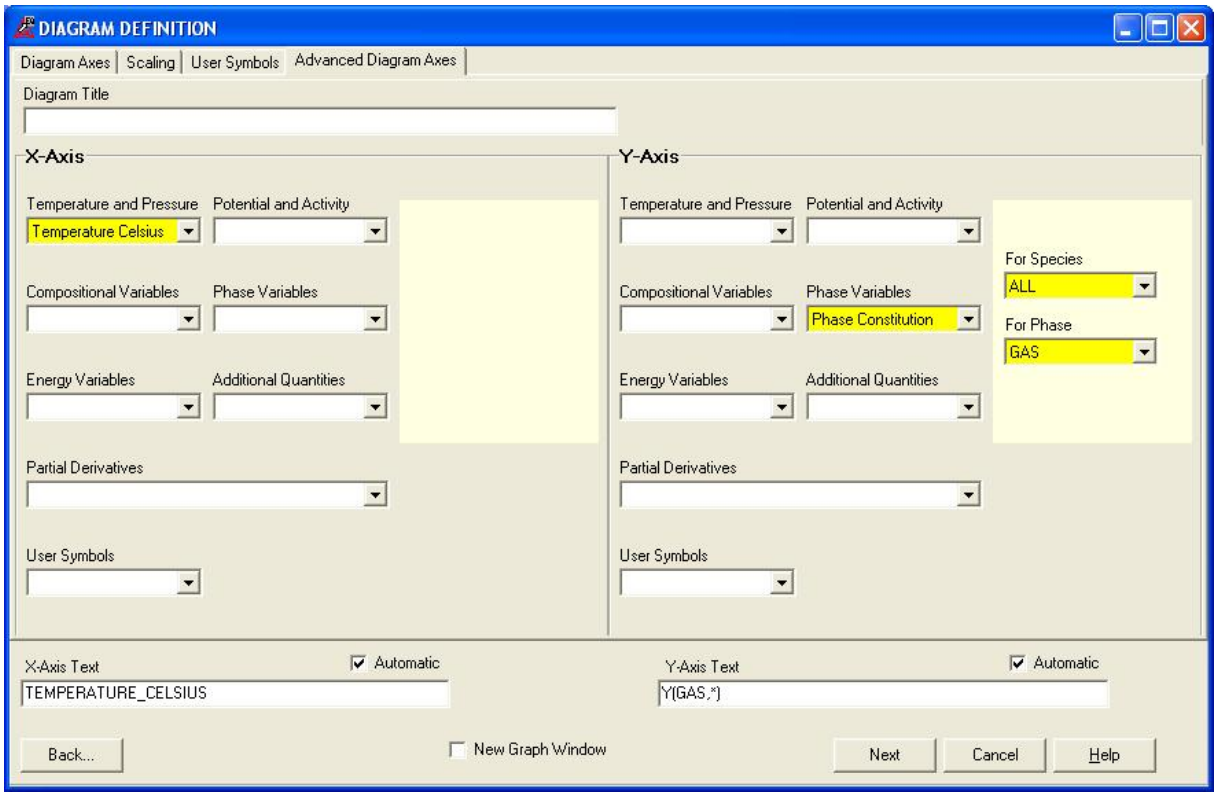
6. Click *Next*. A stepping calculation is performed and the DIAGRAM DEFINITION window appears. The default axes are *Temperature Celsius* and *Phase Fraction* for *all* phases. Keep these axes and click *Next*.



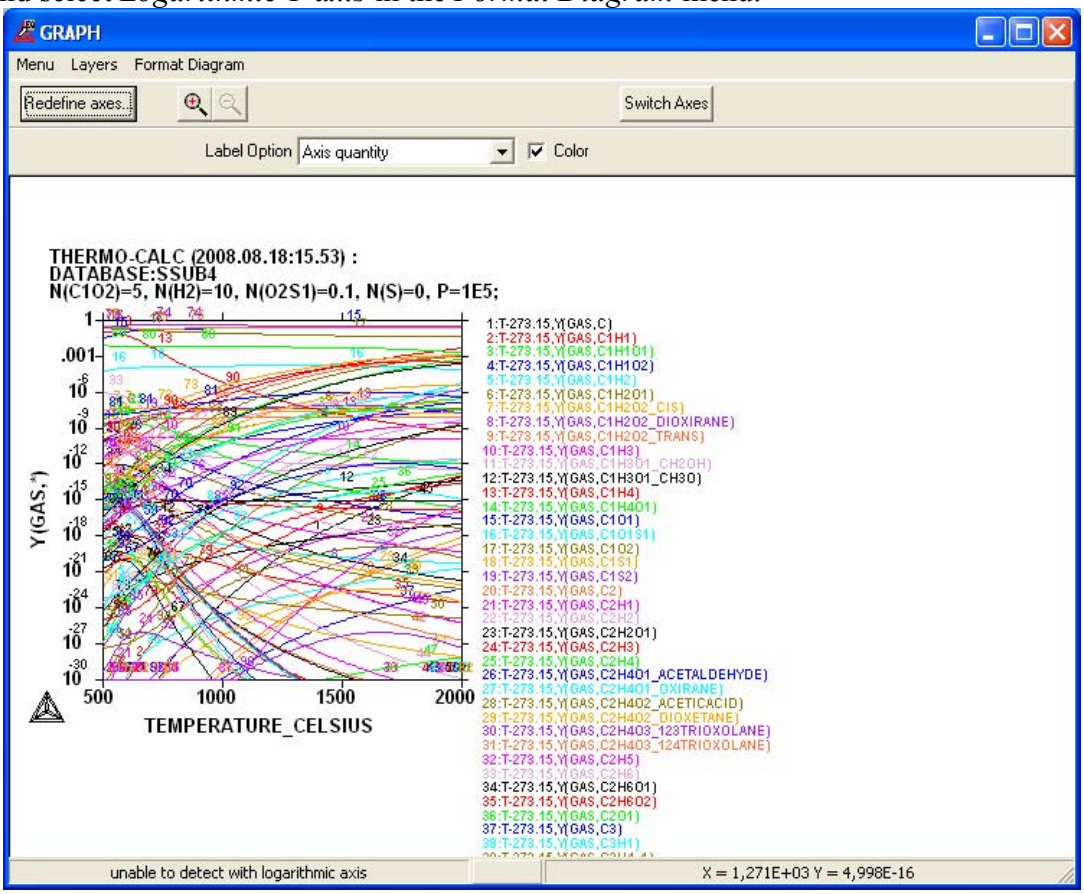
7. Click *Next* to plot the diagram. Choose *Logarithmic Y-axis* in the *Format Diagram* menu. Select *Axis quantity* in the *Label Option* menu and check the *Color* box.



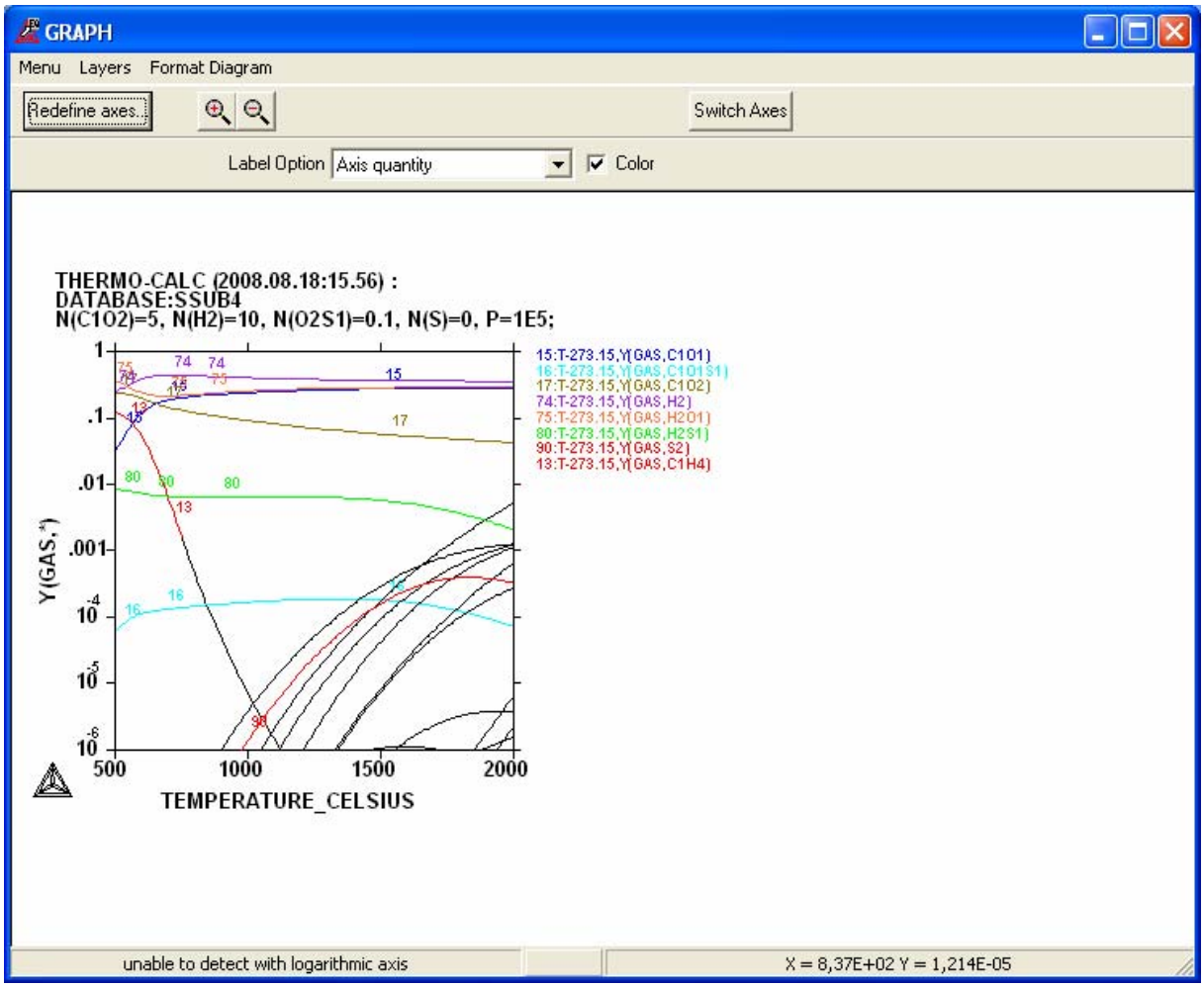
8. Click *Redefine*. Go to the *Advanced Diagram Axes* tab and select *Phase Constitution* for *all* species in the *GAS* phase as the Y-axis.



9. 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.



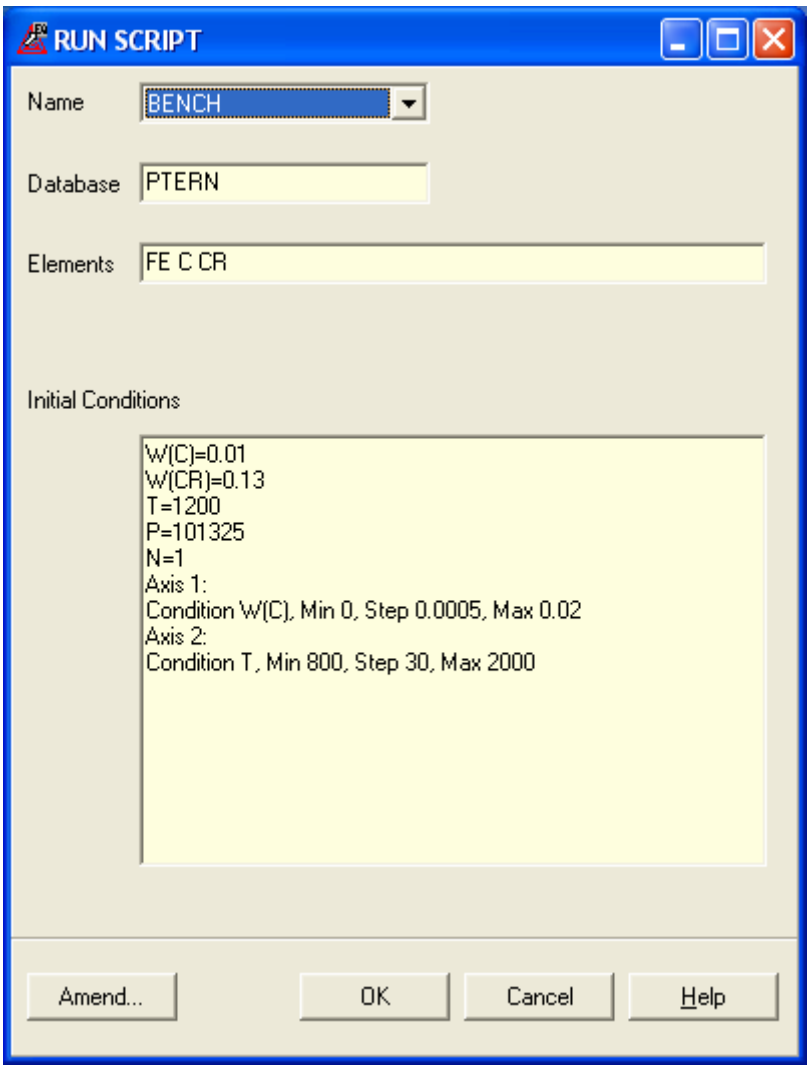
10. Choose *Scaling...* from the *Format Diagram* menu. Change the Min value to *1E-6* and Max to *1* on the *Y-Axis* panel. Click next to plot.



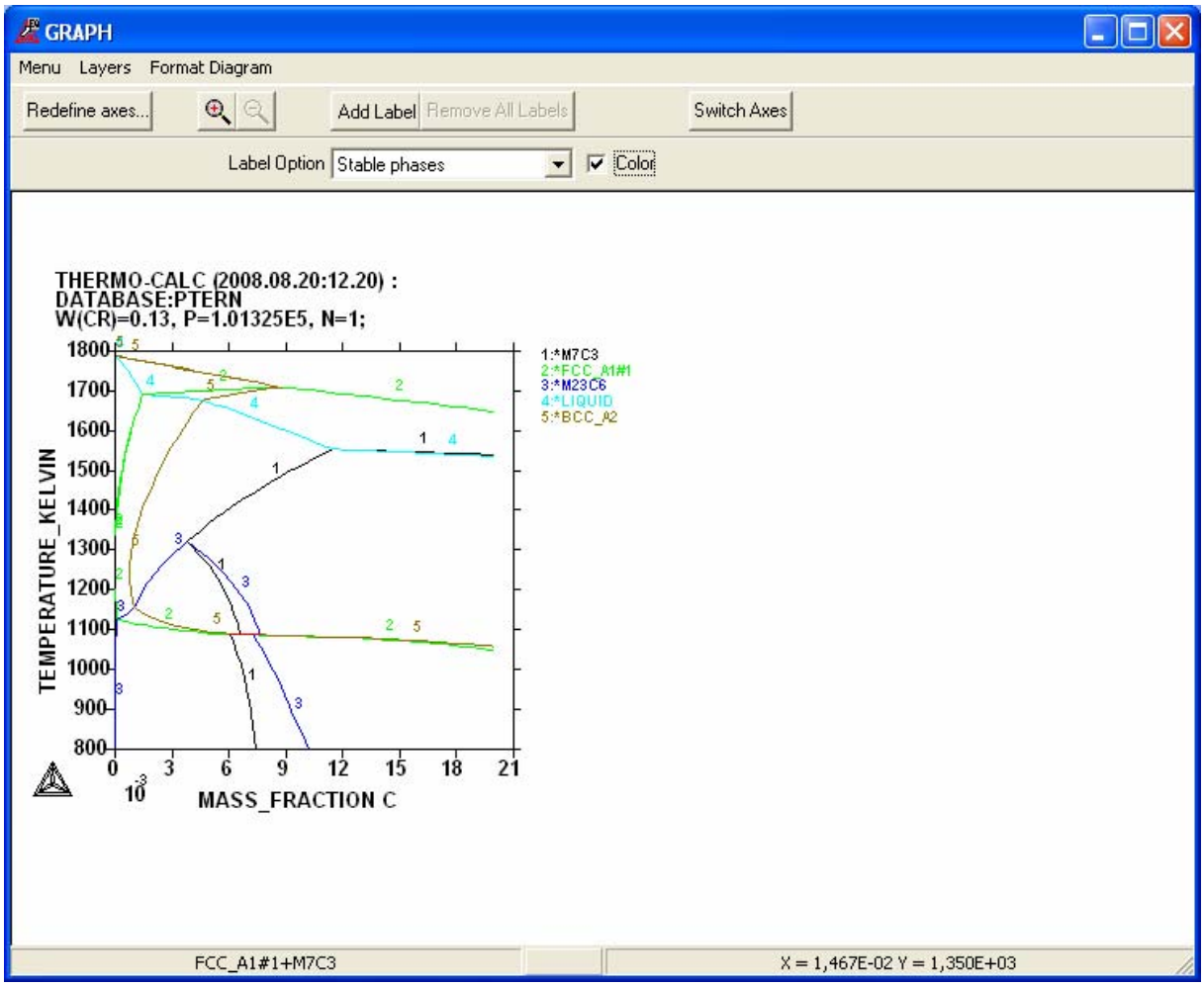
18 Calculation Using Script and how to Implement a Figure to a Word/PowerPoint file

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*.



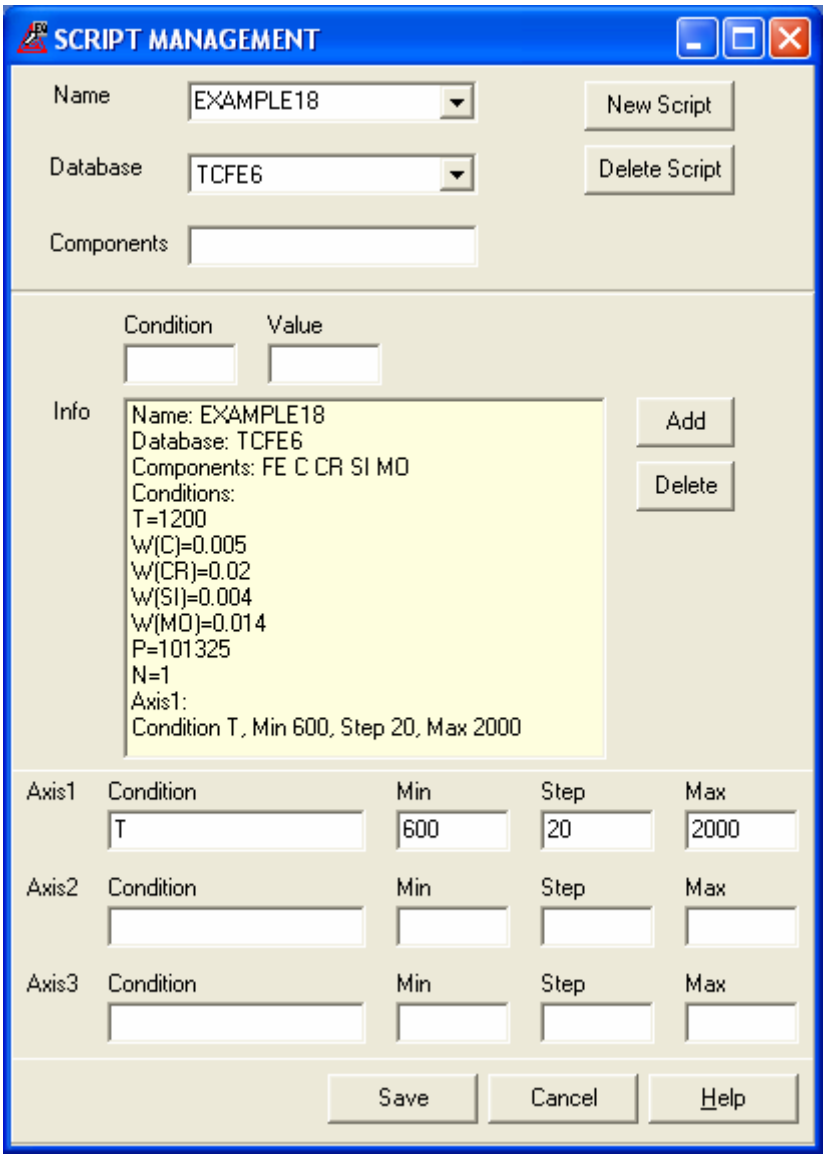
3. Select *Stable phases* in the *Label Option* menu and check the *Color* box.



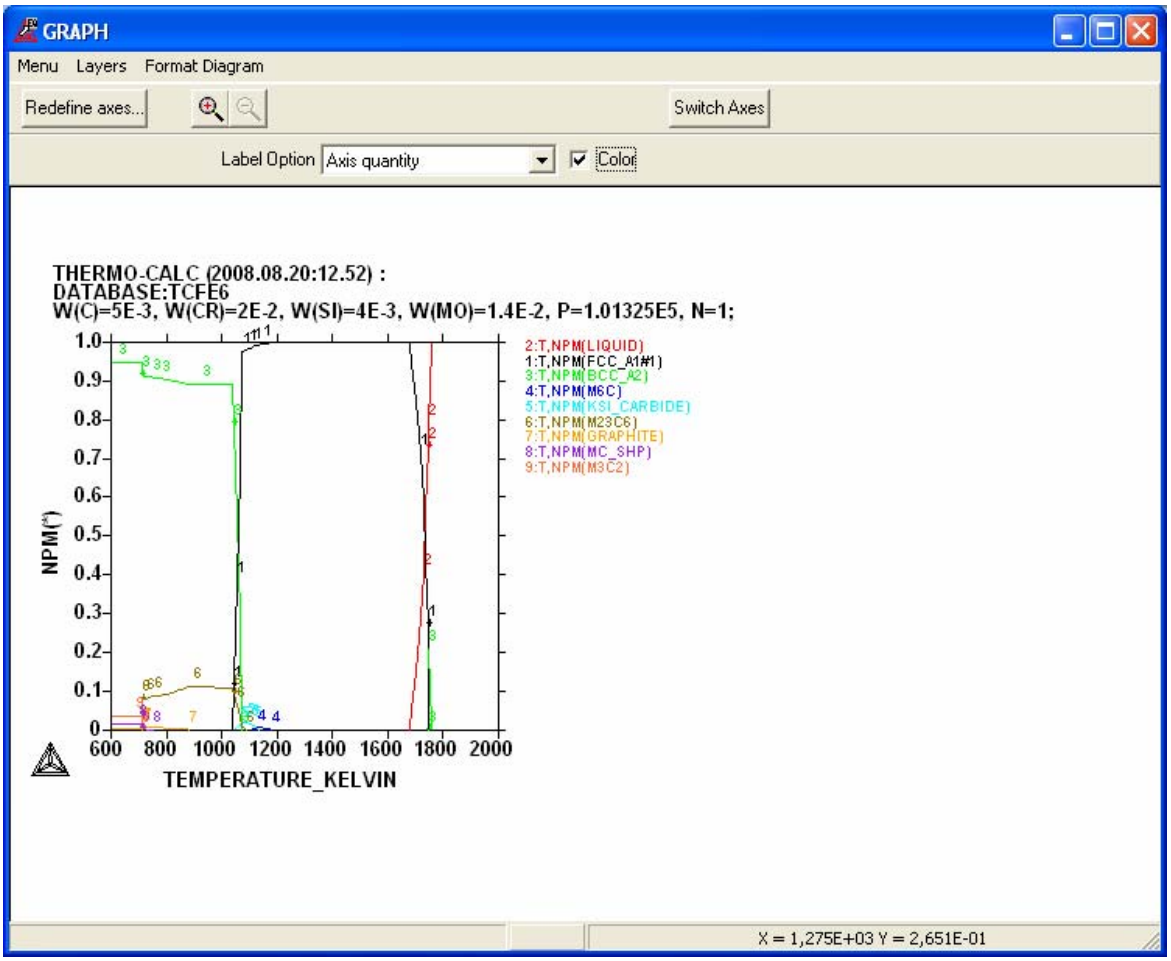
4. To create your own Script select *Script Management* under the *Script* tab in the MAIN window. Click on *New Script*.

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.

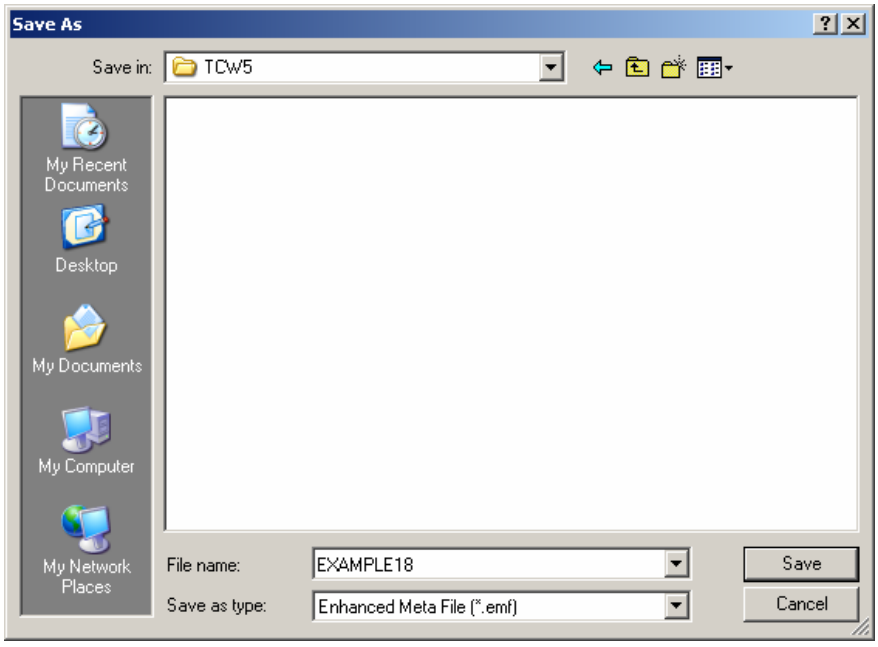
6. Enter T as *Condition* for *Axis 1* with min 600 and max 2000 with a step length of 20. Click *Save*.



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.



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



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