T1: INTRODUCTION TO THE MATCALC GRAPHICAL USER INTERFACE (GUI)

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: none

This first tutorial provides a brief tour of MatCalc's user interface and explains how to perform basic file operations.

CONTENTS

- Appearance of the graphical user interface
- Menus and toolbar
- Console window
- Command history
- Configuring the layout of the GUI
- The 'File' menu
- Creating a new workspace file
- Modifying the working directory
- Adding workspace information
- Saving and closing files
- Getting help

THE GRAPHICAL USER INTERFACE

SCREEN LAYOUT

When MatCalc is first opened, the screen appears as shown below (Windows version).
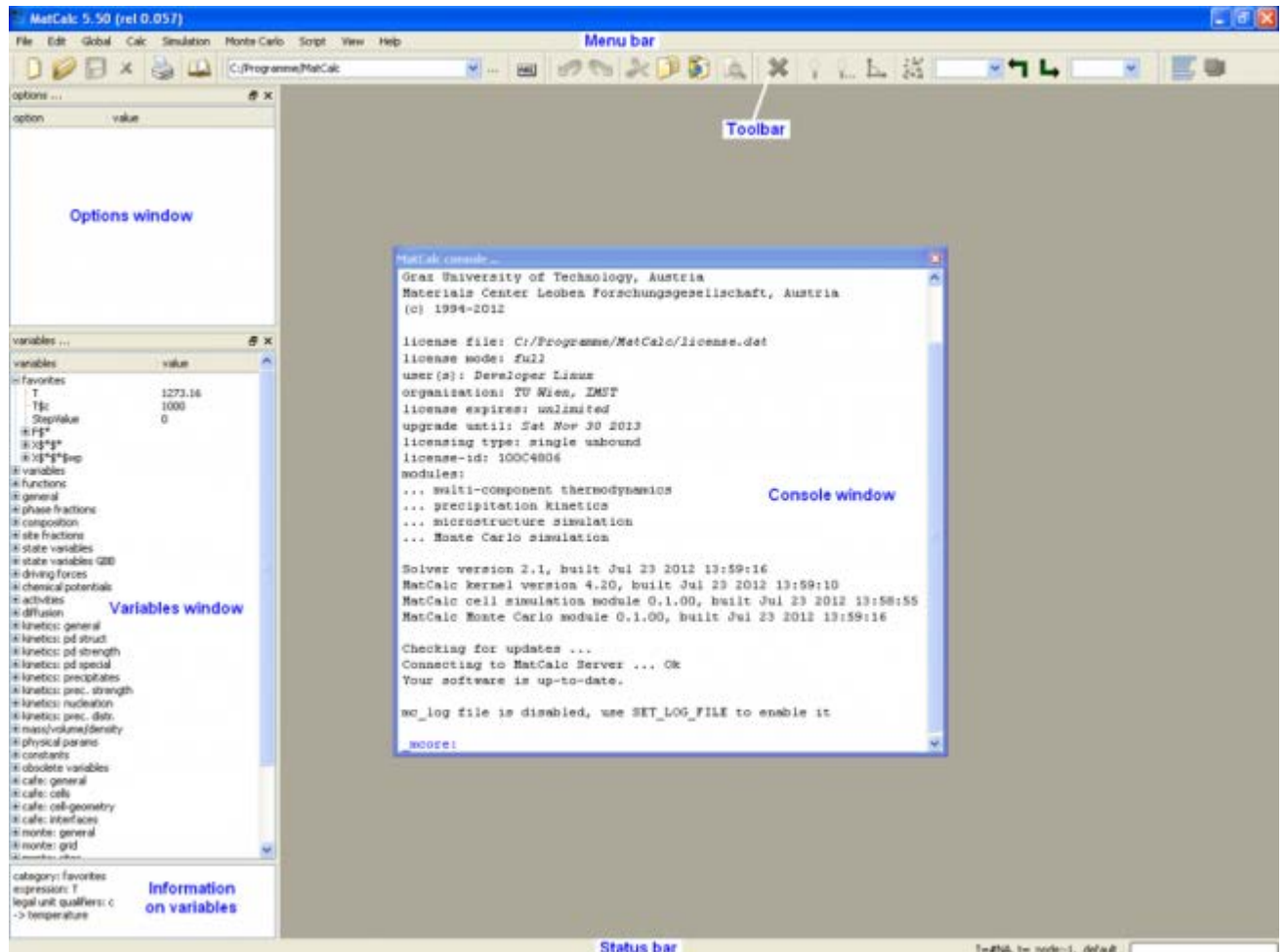
The table below gives brief descriptions of the different areas of the screen.

Menu bar	The main menu (see below).
Toolbar	Icons giving quick access to frequently used functions (see below)
Console	Window for entering command-lines; more information is given below and in Tutorial 12.
Options window	Context-sensitive options to change the way information is displayed. Tutorial 2, Tutorial 4 and Tutorial 5 give more information about the Options window.

Variables window	A list of MatCalc's built-in variables with their current values. See Tutorial 4 and Tutorial 5 for more about variables.
Information on variables	Notes on the currently highlighted entry in the variables window (meaning of variable, units, etc.).
Status bar	Gives information on the current state of the system (temperature, time, etc.) and on the contents of graphical windows (see Tutorial 4).

MENU BAR

As with any typical GUI application, this gives access to a number of sub-menus. The **'File'** and **'Help'** menus are documented in this tutorial, and the contents of the other menus will be described in more detail in subsequent tutorials.

'File': opening, saving and closing files (see **'File operations'** below)

'Edit': text-editing commands such as undo, redo, cut, copy, paste

'Global': commands for setting up the system

'Calc', 'Simulation', 'Monte Carlo': commands for starting various types of calculation

'Script': to run scripts (more on this in Tutorial 13)

'View': to configure the GUI and create new windows for the display of results

'Help': see **'Getting help'** below

TOOLBARS

The toolbar area contains a number of icon groups:

'File etc'

L-R : New file, open, save, close, print, help

'Toolbar'

L-R: Choose working directory, launch script

'Edit'

L-R: Undo, redo, cut, copy, paste, search

'Calculation'

L-R: Stop, Single equilibrium, stepped equilibrium, search phase boundary, precipitation

calculation, choose calculation state, load into calculation state, load into buffer, choose buffer.

'Manage windows'

L-R: Show console, create new window

Right-clicking on the toolbar area gives a menu allowing the user to control which windows and which icon groups are to be displayed on the screen:

COMMAND HISTORY

The command history window can be made to appear by selecting its entry in the menu shown on the picture above or by pressing **'Ctrl' + 'Arrow up'** after clicking on the console window. It gives a chronological list of all the commands entered in the Console.
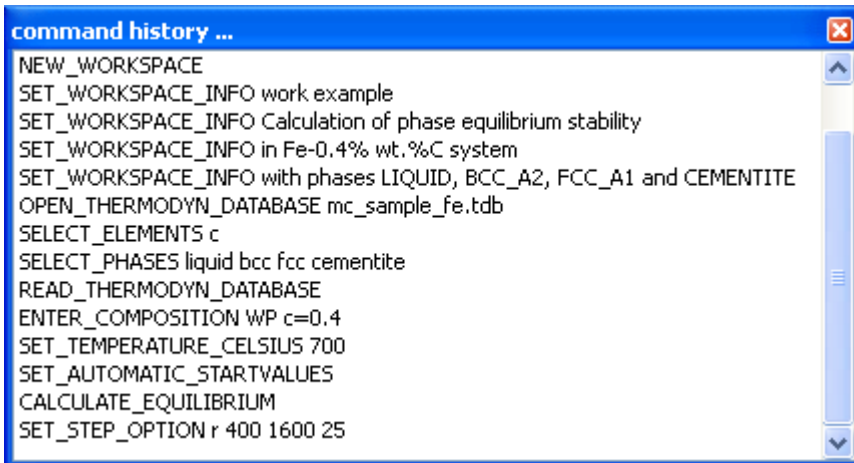
A command can be selected using the mouse pointer or arrow keys. Right-clicking on the command displays the following menu. On the right-hand side of the menus in MatCalc are keyboard shortcuts for the more commonly used commands. It can be seen from the image below that it is sufficient to press the **'Enter'** key to execute the selected command.

Previously used commands can also be accessed in the Console window itself; pressing the up-arrow key displays the most recently entered command, and pressing it repeatedly scrolls through recent commands in reverse chronological order. The command displayed can be edited then executed by pressing the **'Enter'** key.
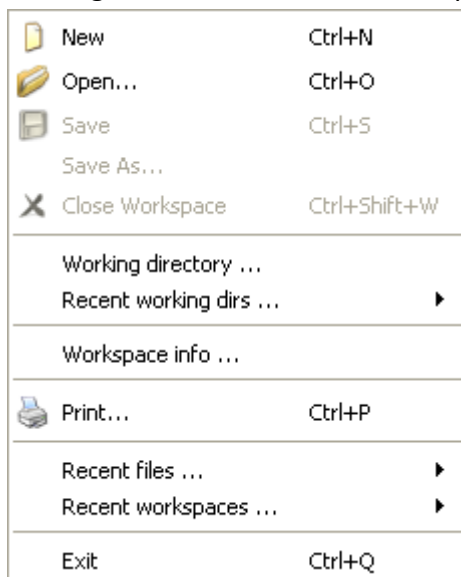
CONFIGURING THE LAYOUT

The icon groups in the toolbar can be rearranged by clicking on the double vertical lines at the left-hand side of the group and dragging to the chosen location. They can be detached from the toolbar area and brought into the currently empty main window area (coloured grey); in this case, they are given title bars similar to that of the **'MatCalc console'**. The Console, Options, Variables and Command History windows can also be attached to or detached from the left-hand column area as required.

FILE OPERATIONS

THE 'FILE' MENU

Clicking on **'File'** in the menu bar opens the following menu:

|		
📄	New	Ctrl+N
📂	Open...	Ctrl+O
💾	Save	Ctrl+S
	Save As...	
✖	Close Workspace	Ctrl+Shift+W
	Working directory ...	
	Recent working dirs ...	▶
	Workspace info ...	
🖨	Print...	Ctrl+P
	Recent files ...	▶
	Recent workspaces ...	▶
	Exit	Ctrl+Q

CREATING A NEW WORKSPACE FILE

The **'workspace'** is the basic file type in MatCalc. It contains all the necessary information on the calculation or series of calculations under consideration, comprising inputs (elements, phases, compositions, thermodynamic and mobility data) and outputs (results of calculations, graphs, etc.). Saving the workspace preserves all this information for future use. Click on the 📄icon or open **'New'** from the **'File'** menu. The following dialogue box will appear:
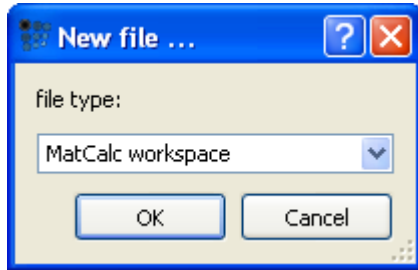
Select **'MatCalc workspace'** from the drop-box. This runs a script file called **'autonew.mcs'**, which makes three additional windows appear: **'Output'**, **'Phase details'** and **'Phase summary'**. When the new workspace is first created, the **'Output'** window displays licence and version information and the **'Phase summary'** and **'Phase details'** windows show messages indicating that no phases have yet been selected. The workspace is now ready for thermodynamic or precipitation calculations to be set up and performed.
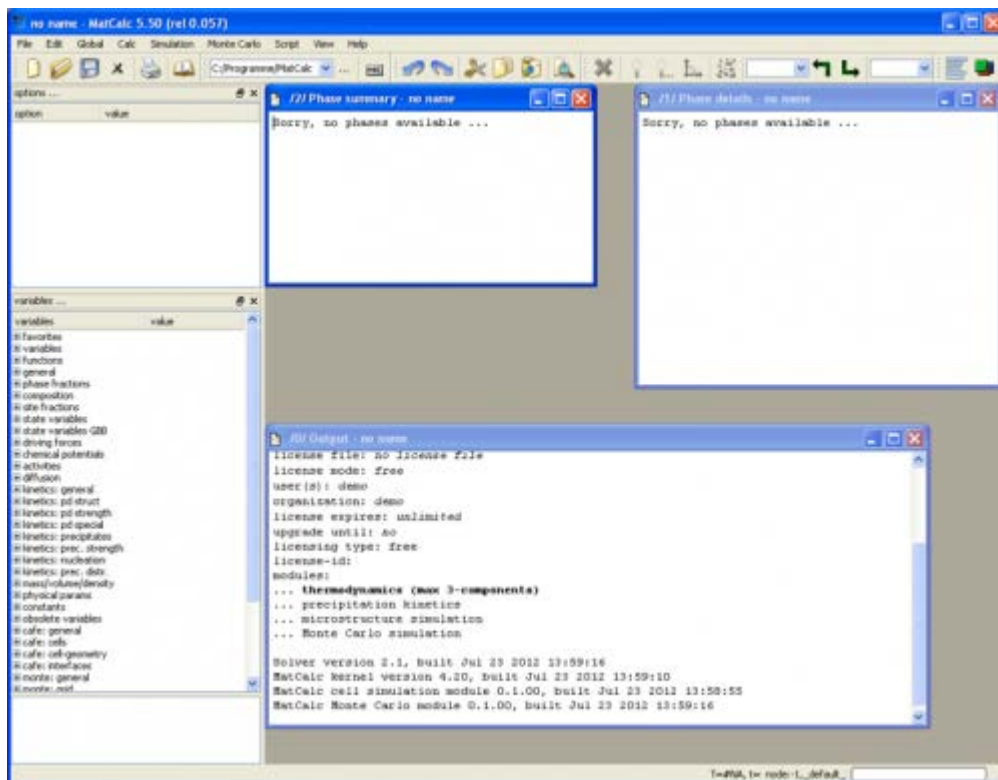

WORKING DIRECTORY

The **'working directory'** is the directory opened by default when saving new files or opening existing ones. Clicking on **'Working directory…'** allows the user to designate an existing directory as the working directory or to create a new directory for this purpose.

The paths of the current working directory and of recently used working directories are listed to the right of **'Recent working dirs…'**, allowing any of these directories to be selected easily.
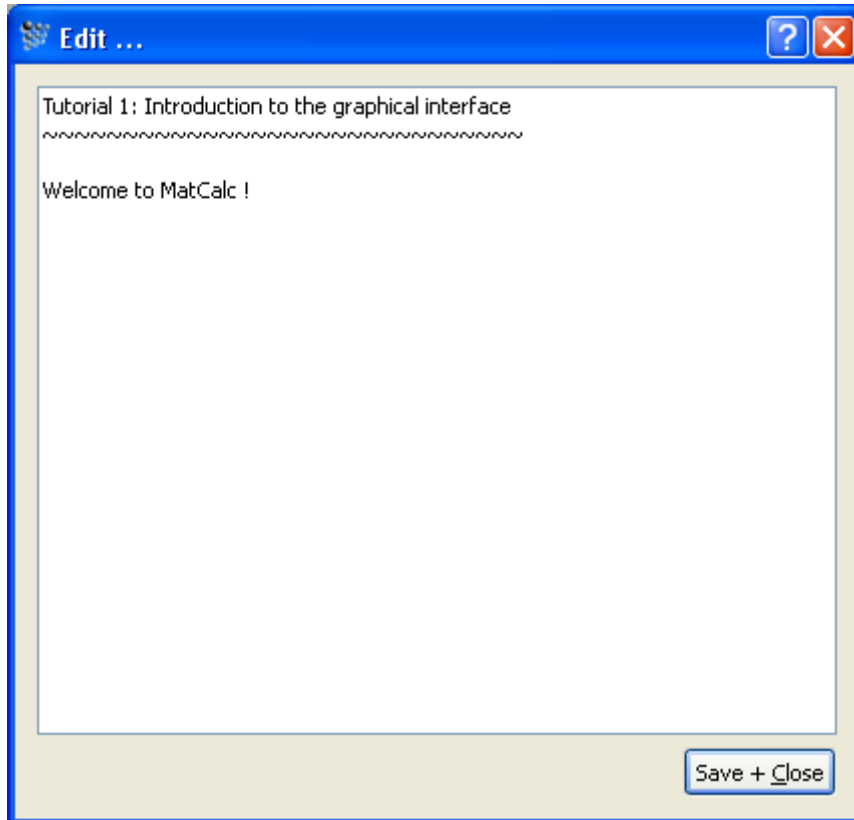

The same information is also available in a drop-box in the toolbar area:
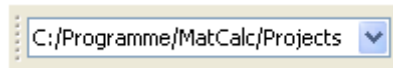
ADDING WORKSPACE INFORMATION

Clicking on **'Workspace info…'** opens a box in which information about the current workspace can be entered. This is useful for details of the assumptions used in the calculation, the sources of experimental data, etc.

SAVE, SAVE AS, CLOSE

Workspaces can be saved using **'Save…'** or **'Save As…'** in the file menu, or the ⊟icon on the toolbar. To close a file, choose **'Close Workspace'** in the file menu or ✕. **Warning: do not close the individual windows on the screen before saving, or their contents will not be saved!**

GETTING HELP

The MatCalc help files are accessible on the web site http://www.matcalc.at → documentation. Presently, no local installation is provided.
In the Console, typing a question-mark will display a list of available commands. These will be discussed more fully in Tutorial 12.

CONSECUTIVE ARTICLES

The tutorial is continued in article T2 - Calculating a single equilibrium

T2: CALCULATING A SINGLE EQUILIBRIUM

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb

This tutorial explains how to determine the equilibrium phases at a given temperature, and their phase fractions and compositions.

CONTENTS

- Opening a database and selecting elements and phases
- Entering a composition
- Calculating an equilibrium at a given temperature
- Interpretation of information displayed in the output, phase summary and phase details windows
- Using the 'Options' window to modify the display
- Phase status indicators
- Calculation states

BEFORE STARTING...

Create a new workspace file (Tutorial 1).

SETTING UP THE SYSTEM

OPENING A THERMODYNAMIC DATABASE AND SELECTING ELEMENTS AND PHASES

In the **'Global'** menu, select **'Databases'**. A window will appear as shown below. The **'Equilibrium database'** box initially displays the message **'database not open…'**. Click on the **'open…'** button; this will open the **'…MatCalc/database'** subdirectory, allowing the user to choose a database. A small database on iron-based materials, **'mc_sample_fe.tdb'**, is provided with MatCalc for demonstration purposes. Select this database and click **'Open'**.
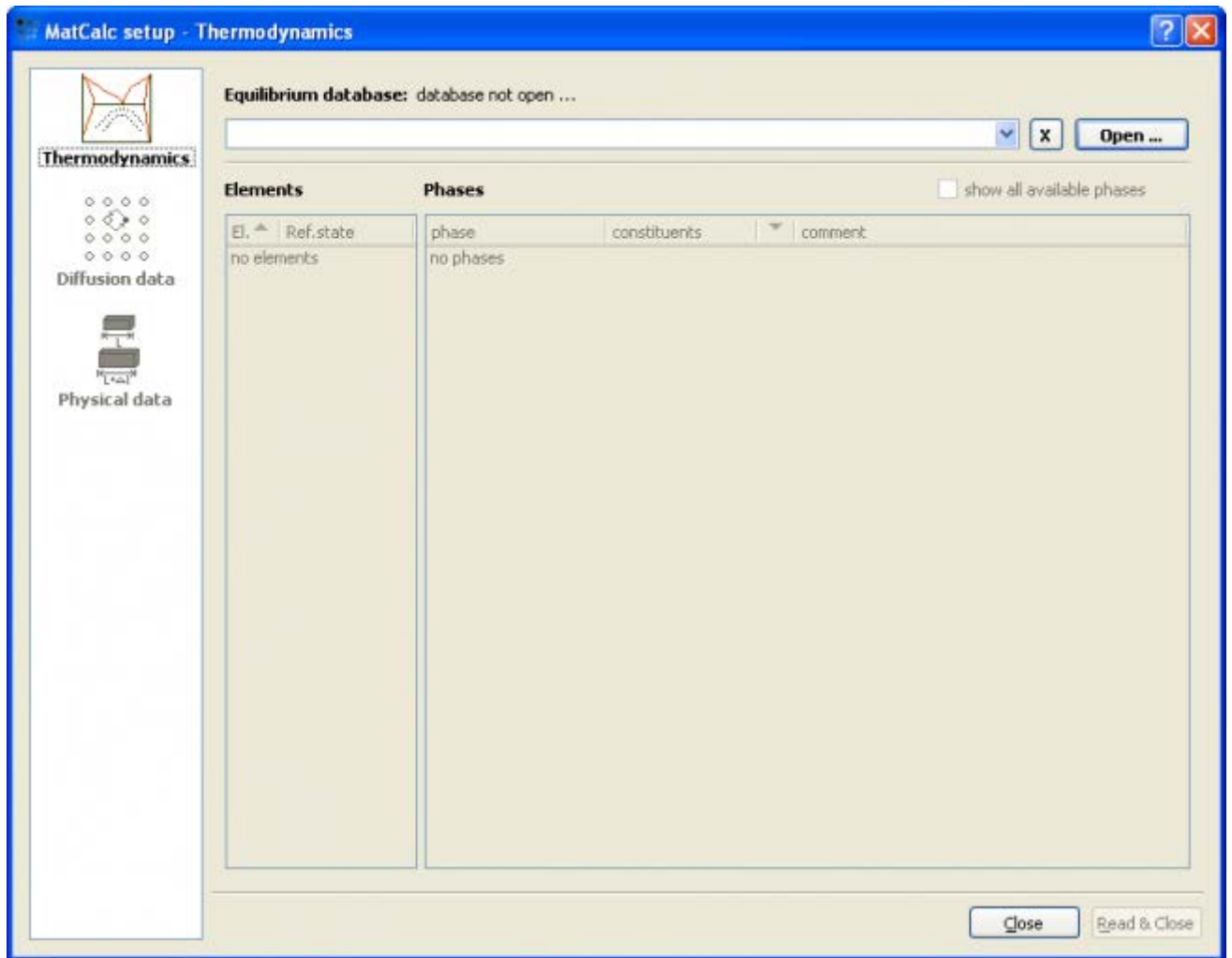
A list of elements will appear in the left-hand box, with FE and VA (vacancies) selected by default. In the right-hand box is a list of the phases which can occur in a system containing the selected elements. Click on **'C'** in the elements box; this will add to the list a number of other phases which can occur in an Fe-C system, such as graphite and several carbides. The **'show all available phases'** box can be used to display all the phases available in the database, irrespective of whether they can form in the system in question.

From the phase list, select **'LIQUID'**, **'BCC_A2'**, **'FCC_A1'**, **'GRAPHITE'** and **'CEMENTITE'**. Phases are described using crystallographic notation: BCC_A2 represents the body-centred cubic phase, which corresponds to ferrite in the iron-carbon system, and FCC_A1 is the face-centred cubic austenite phase in Fe-C. Click **'Read & Close'**.
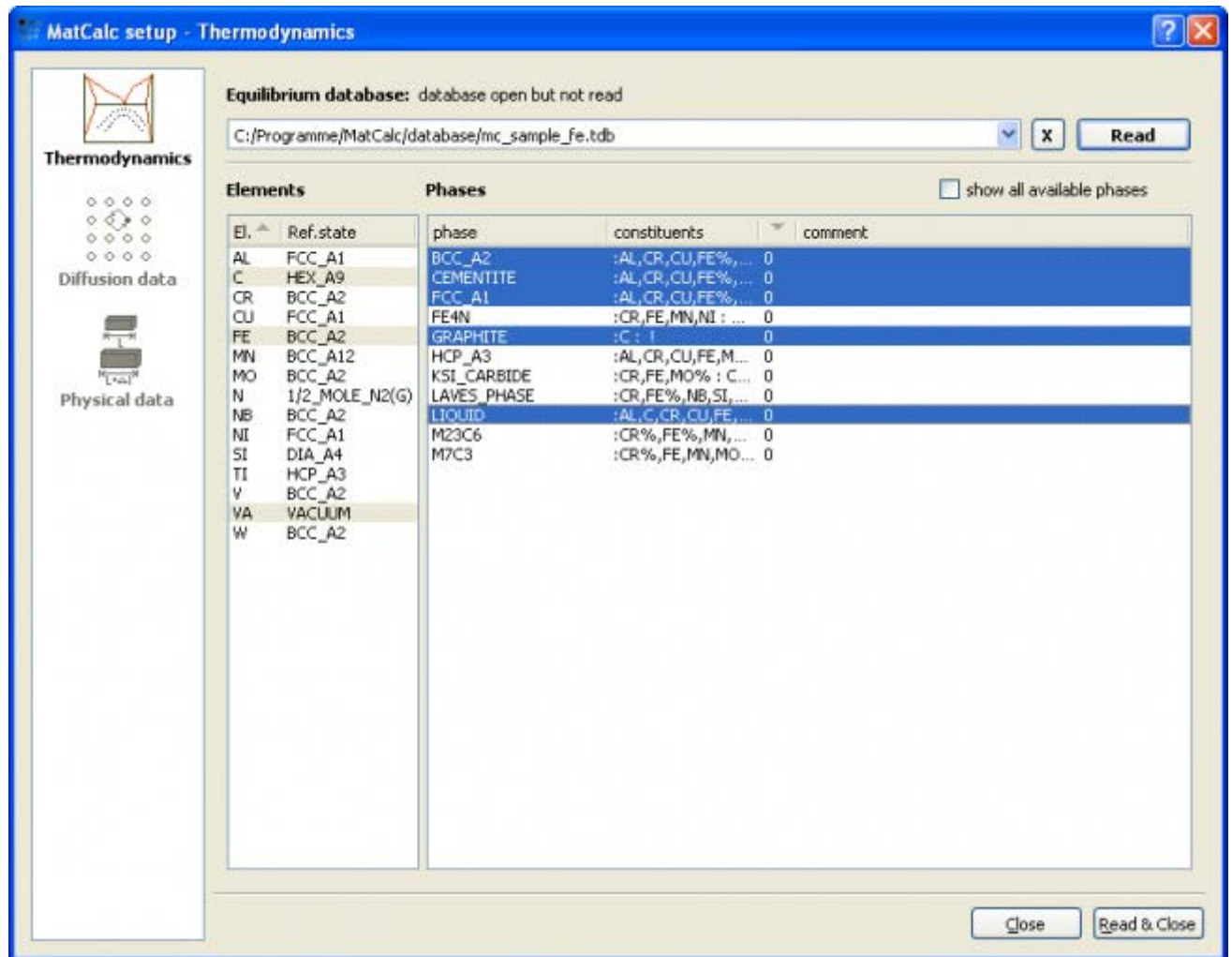
ENTERING THE COMPOSITION

In the **'Global'** menu, select **'Composition'**. This opens the **'System composition'** box. The lower part of the box gives options for the units in which the composition is to be displayed: mole fraction, weight fraction, u-fraction or weight percent. One of the elements, usually the one with the highest mole fraction, is designated as the **'reference element'**, and the amount of this element is calculated as **1-(sum of the amounts of all other elements)** for compositions expressed in fractional form, or **100-(sum of the amounts of all other elements)** for compositions expressed as percentages.

Iron is set as the reference element by default in the 'mc_sample_fe.tdb' database, as can be seen from the **'Ref. Elem'** column in the composition dialogue box. Another element can be set as the reference by selecting the element name and clicking on the **'Set reference element'** button on the right, or by double-clicking in the **'Ref. Elem'** column by the side of the element name.

To enter a composition of **0.4 wt.% C**, select **'weight percent'** as the unit, then highlight element C. Double-click in the **'Amount'** column, click on the **'Change'** button or press **F2** to modify the composition, then type in **'0.4'** and press **'Enter'**.

The system is now ready to perform an equilibrium calculation.
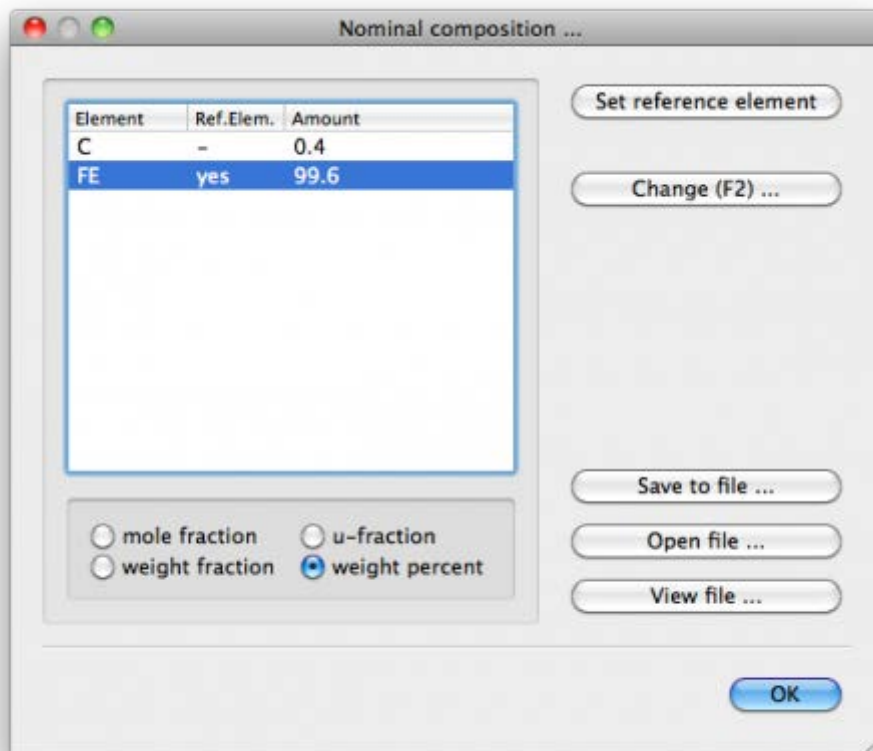
CALCULATING AN EQUILIBRIUM

From the **'Calc'** menu, select **'Set start values'**. This initialises the calculation variables with reasonable values in order to help the Gibbs free energy minimiser to find a solution which satisfies all the boundary conditions. This command is useful if the solution algorithm seems to be 'stuck' and unable to find an equilibrium.

Once one valid equilibrium has been found, solutions at other temperatures or boundary conditions are much easier to obtain. From the **'Calc'** menu, select **'Equilibrium'**, or click on the icon in the toolbar.

The following window appears:
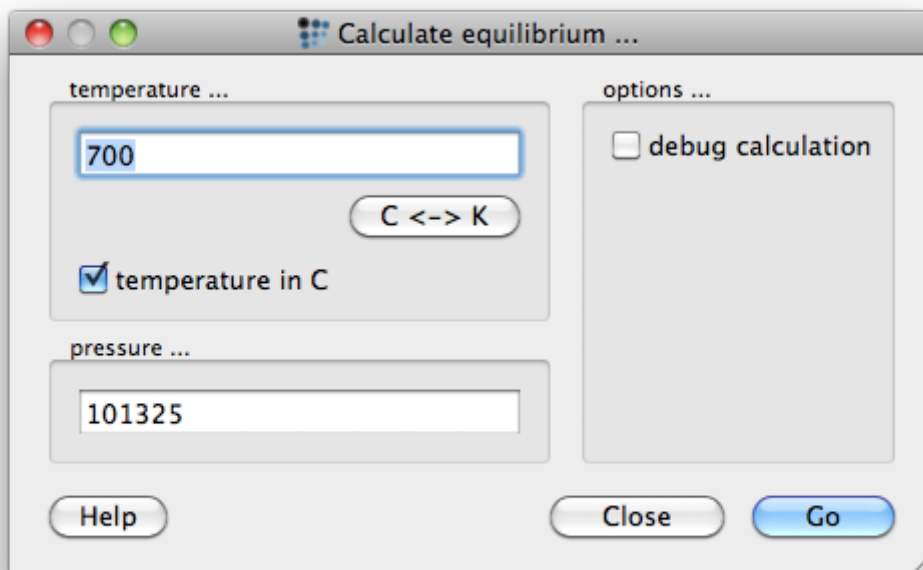
Enter **'700'** in the temperature box and ensure that **'temperature in C'** is selected. Leave the pressure at its default value. Click on **'Go'** to start the calculation.

INTERPRETING THE RESULTS OF THE CALCULATION

The **'Output'**, **'Phase status'** and **'Phase details'** windows each show information on the calculation which has just been performed. The final three lines of the Output window list the number of iterations, the calculation time, the temperature and the Gibbs energy of the system. The **'- OK -'** message in the final line indicates that the calculation was successful, with no errors reported. If any errors do occur, the message **'*** error ***'** followed by a description of the nature of the error will be displayed instead of the **'OK'** message. In this case, reset the calculation with **'Set start values'** and repeat it using **'Equilibrium'**. It is always advisable to check the status of the calculation in the Output window before proceeding.
The other lines visible in the Output window are messages relating to the opening and reading of the thermodynamic database.

```
modules:
... thermodynamics (max 3-components)
... precipitation kinetics
... microstructure simulation
... Monte Carlo simulation

Solver version 2.1, built Aug  7 2011 20:22:22
MatCalc kernel version 4.20, built Aug  7 2011 20:21:52
MatCalc cell simulation module 0.1.00, built Aug  7 2011 20:22:09
MatCalc Monte Carlo module 0.1.00, built Aug  7 2011 20:22:11
opening database '/Applications/MatCalc/database/mc_sample_fe.tdb' ... - OK -
reading thermodynamic data '/Applications/MatCalc/database/mc_sample_fe.tdb' ...
collecting symbols '/Applications/MatCalc/database/mc_sample_fe.tdb' ...
elements: VA C FE
phases: LIQUID FCC_A1 BCC_A2 CEMENTITE GRAPHITE
Gibbs: 5 Phases / 0 Composition-Set(s) created
Gibbs: 30 functions linked ...
Gibbs: T = 1273.160000 K, P = 101325.000000 Pa, moles = 1

iter: 54, time used: 0.09 s
T:  700 C (973.16 K), GibbsEnergy: -39976.445 J
- OK -
```

Information on the phase stabilities is shown in the **'Phase summary'** window. Those phases with non-zero phase fractions are termed **'active'** and are listed in the first block. Inactive phases (those which are unstable, with negative driving forces) are listed in the second block. The third column gives the phase fraction and the column after **'dfm:'** gives the driving force in J/mole. It can be seen that BCC_A2 (ferrite) and GRAPHITE are the stable phases at 700°C.


```
BCC_A2          *        act        9.82166e-01  dfm: +0.00000e+00
GRAPHITE                 act        1.78337e-02  dfm: +0.00000e+00

### inactive ###
FCC_A1                 - OK -       0.00000e+00  dfm: -1.88360e+02
CEMENTITE              - OK -       0.00000e+00  dfm: -5.82261e+02
LIQUID                 - OK -       0.00000e+00  dfm: -4.07902e+03
```

The **'Phase details'** window provides more comprehensive information on the properties of the phases, including the molar Gibbs free energy of the phase (the number after **'gm:'**) and the phase compositions (expressed in mole fraction by default), as well as the information provided in the 'Phase summary'. The phases are again grouped according to whether they are active or inactive.

```
####  /BCC_A2/ moles: 0.982166, gm: -40484.2 (-40484.2), sff: 0.999494
Phasestatus: entered - active
FE +9.99494e-01    C +5.06362e-04

####  /GRAPHITE/ moles: 0.0178337, gm: -12010.7 (-12010.7), sff: 1
Phasestatus: entered - active
 C +1.00000e+00


### inactive ###

####  /FCC_A1/ moles: 0, gm: -39544.4 (-39544.4), sff: 0.973115
Phasestatus: entered - not active (dfm=-188.4)
FE +9.73115e-01    C +2.68849e-02

####  /CEMENTITE/ moles: 0, gm: -32794.4 (24703.1), sff: 0.25
Phasestatus: entered - not active (dfm=-582.3)
FE +7.50000e-01    C +2.50000e-01

####  /LIQUID/ moles: 0, gm: -32172 (-32172), sff: 1
Phasestatus: entered - not active (dfm=-4079)
FE +8.50899e-01    C +1.49101e-01
```

USING THE 'OPTIONS' WINDOW TO MODIFY THE DISPLAY

To change the units in which the composition is displayed in the **'Phase details'** window, first highlight this window and then go to the **'Options'** window. (If this is not shown on the screen, make it appear by selecting **'View > Show options window'** or right-clicking in the toolbar area and selecting **'options'** from the menu.)

The **'Options'** window provides display options for the currently highlighted window. In the case of the **'Phase details'** window, the composition can be displayed as a mole fraction, a weight fraction or a u-fraction, and can also be expressed as a percentage if required.
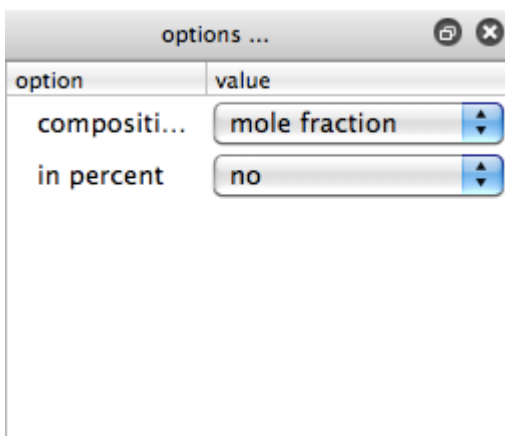
PHASE STATUS: SUSPENDED AND DORMANT PHASES

The calculation has shown that at 700°C, BCC_A2 (ferrite) and graphite are the equilibrium (i.e. most thermodynamically stable) phases. However, it is observed in practice that in Fe-C systems with relatively low carbon contents, graphite formation is extremely slow, and can be considered not to occur over practical timescales.

Since this is the case, it is useful to calculate a metastable equilibrium, for which graphite formation is not allowed. Go to **'Global > Phase status'** and highlight **'GRAPHITE'**. In the **'General'** tab, the uppermost section is labelled **'Flags…'**. Click to place a tick in the box next to **'suspended'**.
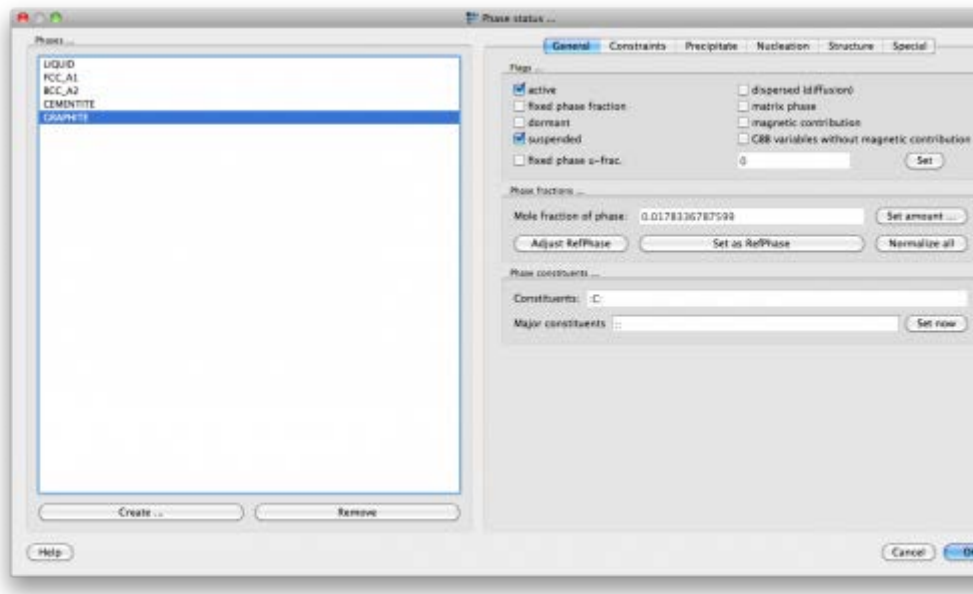
Repeat the equilibrium calculation and note the difference in results in the **'Phase summary'** window:

```
BCC_A2        *      act       9.29184e-001      dfm: +0.00000e+000
CEMENTITE            act       7.08157e-002      dfm: +0.00000e+000
### inactive ###
FCC_A1               - OK -    0.00000e+000      dfm: -1.19832e+002
LIQUID               - OK -    0.00000e+000      dfm: -3.71990e+003
### suspended ###
GRAPHITE
```

Now BCC_A2 and CEMENTITE are active, FCC_A1 and LIQUID are inactive and GRAPHITE is listed as **'suspended'**. Suspending a phase causes the program to consider it as if it were not there at all; the next most stable phase (in this case, cementite) becomes the equilibrium phase. Alternatively, the flag can be set to **'dormant'** using the same procedure. In this case, the phase is considered not to appear, but its driving force is still evaluated. In this case, cementite does not become active, as shown by the results below:

```
BCC_A2            *      act       9.82166e-001      dfm: +0.00000e+000
### inactive ###
GRAPHITE              dorm.    1.78337e-002      dfm: +0.00000e+000
FCC_A1               - OK -    0.00000e+000      dfm: -1.88360e+002
CEMENTITE            - OK -    0.00000e+000      dfm: -5.82261e+002
LIQUID               - OK -    0.00000e+000      dfm: -4.07902e+003
```

In order to eliminate graphite completely from the system, it is necessary to re-load the thermodynamic data from the database. Re-open **'Global > Databases'** and click on **GRAPHITE** to unselect it, then click on **'Read & Close'**. A warning will appear, stating that all existing data will be deleted. Accept this by clicking on **'Yes'**. A new message, with updated information on

the thermodynamic data, appears in the **'Output'** window. Reading in new data from the database erases any previous equilibrium calculation results, so repeat the equilibrium calculation at 700°C to obtain an equilibrium without graphite (if you get an error message, click on **'Set start values'** in **'Calc'** menu). The driving forces obtained should be identical to those found in the previous calculation in which graphite was suspended:

```
BCC_A2   *   act   9.29184e-001   dfm: +0.00000e+000
CEMENTITE   act   7.08157e-002   dfm: +0.00000e+000
inactive
FCC_A1   - OK -   0.00000e+000   dfm: -1.19832e+002
LIQUID   - OK -   0.00000e+000   dfm: -3.71990e+003
```

### CALCULATION STATES

By default, the results from a previous equilibrium calculation are overwritten when a new calculation is carried out. However, it is sometimes useful to store the results from a calculation for future use. The **'Calculation states'** feature is provided for this purpose; it can be found in the **'Global'** menu under **'CalcStates'**. In the sub-menu, click on **'Create'** and type the name in the box:
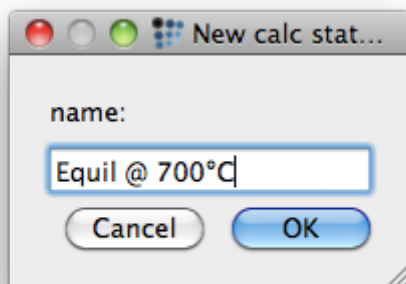


The calculation state stores all information on an equilibrium including the complete phase status, composition and any compositional states which may apply. Calculate another equilibrium at 600°C and store it in another calculation state. These states are now both available in the calculation state drop-box on the toolbar:
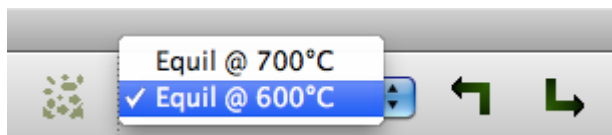


Select a calculation state from this box and load the stored equilibrium with the  button (This can also be done using **'Global > CalcStates > Select'** and then **'Load'** ). Note how the contents of the **'Phase details'** and **'Phase summary'** windows are immediately updated with the results stored in the calculation state, and the temperature at which the equilibrium was calculated is shown in the status bar towards the bottom right of the screen. The results of the current equilibrium calculation can be saved into an existing calculation state by selecting

the name of the state in the drop-box and then clicking on the  button or using **'Global >**

**CalcStates > Select'** and then **'Save'. NB: Calculation states, like all other calculation results, are erased when data is re-read from the database!**

To finish…

Save the workspace using **'File > Save as…'**. Workspace files are automatically given the file extension **'.mcw'**.

Consecutive articles

The tutorial is continued in article T3 - Performing a stepped equilibrium calculation.

## T3: STEPPED EQUILIBRIUM CALCULATIONS

*This tutorial was tested on*
*MatCalc version 5.50 rel 0.057*
*license: free*
*database: mc_sample_fe.tdb*

### CONTENTS

- Re-opening a saved file and loading a calculation state
- Calculating a stepped equilibrium with varying temperature
- Understanding the results in the Output window
- Working with multiple buffers
- Calculating a stepped equilibrium with varying composition
- The "Edit buffer states" window

### BEFORE STARTING…**

Re-open the file saved from Tutorial 2 and load the calculation state **'Equil @ 600°C'**.

### STEPPED EQUILIBRIUM CALCULATION WITH VARYING TEMPERATURE

### RUNNING THE STEPPED CALCULATION

Select **'Stepped calculation…'** from the **'Calc'** menu or click on the 💡icon. The **'Step equilibrium'** window will appear. Select **'Temperature'** (the uppermost choice in the left-hand column).

In the **'Range'** box, the default **'Start'**, **'Stop'** and **'Step interval'** values are 400, 1600 and 25 respectively. Keep these values and verify that the **'Temperatures in Celsius'** option has been selected. The step direction is unimportant, and it is not necessary to enter the interval as **'-25'** if stepping in a negative direction. The contents of the **'Vary'** and **'Boundary conditions'** boxes are currently greyed-out because they are not applicable to a temperature-step calculation. Click on the **'Go'** button at the bottom right of the window.
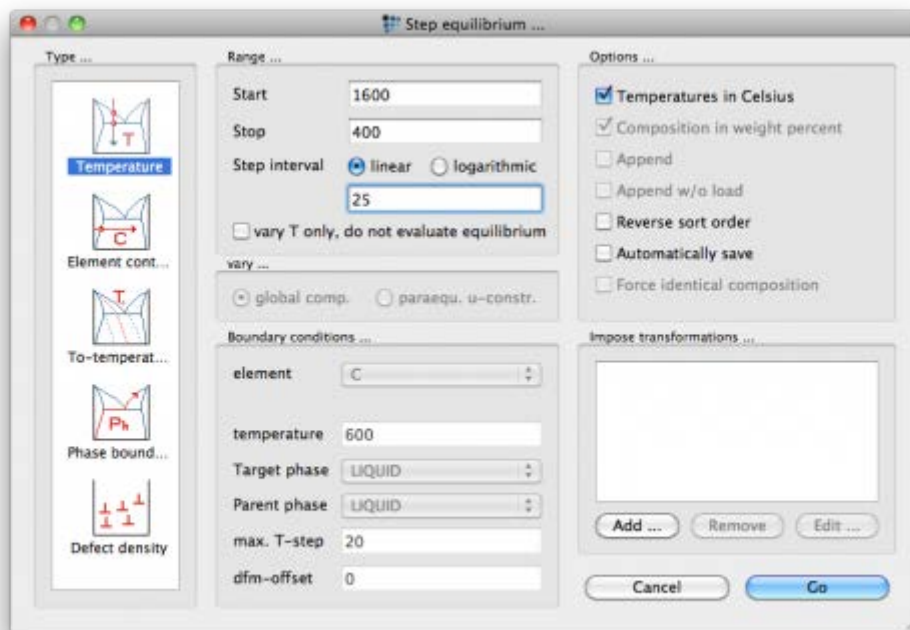
## OUTPUT

The **'Output'** window should show the following series of messages:

```
1, 0.00 s, 600.00 C (873.16 K), its 2, BCC_A2 CEMENTITE - OK -
2, 0.00 s, 625.00 C (898.16 K), its 4, BCC_A2 CEMENTITE - OK -
3, 0.00 s, 650.00 C (923.16 K), its 4, BCC_A2 CEMENTITE - OK -
4, 0.00 s, 675.00 C (948.16 K), its 4, BCC_A2 CEMENTITE - OK -
5, 0.00 s, 700.00 C (973.16 K), its 4, BCC_A2 CEMENTITE - OK -
6, 0.02 s, 725.00 C (998.16 K), its 4, BCC_A2 CEMENTITE - OK -
Tsol 'FCC_A1': 726.62 C (999.78 K) iter: 4, time used: 0.00 s
Tsol 'CEMENTITE': 726.62 C (999.78 K) iter: 5, time used: 0.00 s
7, 0.05 s, 750.00 C (1023.16 K), its 5, FCC_A1 BCC_A2 - OK -
8, 0.02 s, 775.00 C (1048.16 K), its 5, FCC_A1 BCC_A2 - OK -
Tsol 'BCC_A2': 787.13 C (1060.29 K) iter: 4, time used: 0.00 s
9, 0.00 s, 800.00 C (1073.16 K), its 4, FCC_A1 - OK -
10, 0.00 s, 825.00 C (1098.16 K), its 2, FCC_A1 - OK -
11, 0.00 s, 850.00 C (1123.16 K), its 2, FCC_A1 - OK -
12, 0.01 s, 875.00 C (1148.16 K), its 2, FCC_A1 - OK -
13, 0.00 s, 900.00 C (1173.16 K), its 2, FCC_A1 - OK -
14, 0.00 s, 925.00 C (1198.16 K), its 2, FCC_A1 - OK -
15, 0.00 s, 950.00 C (1223.16 K), its 2, FCC_A1 - OK -
16, 0.00 s, 975.00 C (1248.16 K), its 2, FCC_A1 - OK -
17, 0.02 s, 1000.00 C (1273.16 K), its 2, FCC_A1 - OK -
18, 0.00 s, 1025.00 C (1298.16 K), its 2, FCC_A1 - OK -
19, 0.00 s, 1050.00 C (1323.16 K), its 2, FCC_A1 - OK -
20, 0.00 s, 1075.00 C (1348.16 K), its 2, FCC_A1 - OK -
21, 0.00 s, 1100.00 C (1373.16 K), its 2, FCC_A1 - OK -
22, 0.00 s, 1125.00 C (1398.16 K), its 2, FCC_A1 - OK -
23, 0.00 s, 1150.00 C (1423.16 K), its 2, FCC_A1 - OK -
24, 0.00 s, 1175.00 C (1448.16 K), its 2, FCC_A1 - OK -
25, 0.00 s, 1200.00 C (1473.16 K), its 2, FCC_A1 - OK -
26, 0.02 s, 1225.00 C (1498.16 K), its 2, FCC_A1 - OK -
27, 0.00 s, 1250.00 C (1523.16 K), its 2, FCC_A1 - OK -
28, 0.00 s, 1275.00 C (1548.16 K), its 2, FCC_A1 - OK -
29, 0.00 s, 1300.00 C (1573.16 K), its 2, FCC_A1 - OK -
30, 0.00 s, 1325.00 C (1598.16 K), its 2, FCC_A1 - OK -
```

```
31, 0.01 s, 1350.00 C (1623.16 K), its 2, FCC_A1 - OK -
32, 0.00 s, 1375.00 C (1648.16 K), its 2, FCC_A1 - OK -
33, 0.00 s, 1400.00 C (1673.16 K), its 2, FCC_A1 - OK -
34, 0.00 s, 1425.00 C (1698.16 K), its 2, FCC_A1 - OK -
35, 0.00 s, 1450.00 C (1723.16 K), its 2, FCC_A1 - OK -
Tsol 'LIQUID': 1453.05 C (1726.21 K) iter: 3, time used: 0.00 s
36, 0.00 s, 1475.00 C (1748.16 K), its 3, LIQUID FCC_A1 - OK -
Tsol 'FCC_A1': 1494.60 C (1767.76 K) iter: 4, time used: 0.00 s
Tsol 'BCC_A2': 1494.60 C (1767.76 K) iter: 5, time used: 0.01 s
37, 0.03 s, 1500.00 C (1773.16 K), its 5, LIQUID BCC_A2 - OK -
Tsol 'BCC_A2': 1505.64 C (1778.80 K) iter: 4, time used: 0.00 s
38, 0.02 s, 1525.00 C (1798.16 K), its 4, LIQUID - OK -
39, 0.00 s, 1550.00 C (1823.16 K), its 2, LIQUID - OK -
40, 0.02 s, 1575.00 C (1848.16 K), its 2, LIQUID - OK -
41, 0.00 s, 1600.00 C (1873.16 K), its 2, LIQUID - OK -
changing step direction ...
42, 0.01 s, 575.00 C (848.16 K), its 5, BCC_A2 CEMENTITE - OK -
43, 0.00 s, 550.00 C (823.16 K), its 5, BCC_A2 CEMENTITE - OK -
44, 0.00 s, 525.00 C (798.16 K), its 5, BCC_A2 CEMENTITE - OK -
45, 0.00 s, 500.00 C (773.16 K), its 5, BCC_A2 CEMENTITE - OK -
46, 0.00 s, 475.00 C (748.16 K), its 5, BCC_A2 CEMENTITE - OK -
47, 0.00 s, 450.00 C (723.16 K), its 5, BCC_A2 CEMENTITE - OK -
48, 0.01 s, 425.00 C (698.16 K), its 5, BCC_A2 CEMENTITE - OK -
49, 0.00 s, 400.00 C (673.16 K), its 5, BCC_A2 CEMENTITE - OK -
50, 0.02 s, 400.00 C (673.16 K), its 2, BCC_A2 CEMENTITE - OK -
Steps: 51, CalcTime: 0.45 s
AktStepVal: 673.160000
- OK -
```

Each line corresponds to an equilibrium calculated at a single temperature value and comprises a line number, the calculation time, the temperature, the number of iterations, the stable phases at that temperature and an **'- OK -'** message indicating that the equilibrium calculation was successful.

Note that the temperature-stepping starts from the equilibrium at 600°C loaded from the calculation state. Initially, the temperature is increased by the **'Step interval'** each time until the upper temperature limit is reached.

Then, a **'changing step direction'** message is displayed and, again starting from the equilibrium at 600°C, the temperature is decreased until the lower limit is reached. Also note the lines beginning with **'Tsol'**: phase solubility temperatures are automatically evaluated during the stepped calculation. Thus it is seen in the output above that from **600°C to 726.62°C**, the two stable phases are **BCC_A2** (ferrite) and **CEMENTITE**. At **726.62°C**, **FCC_A1** (austenite) becomes stable, and cementite becomes unstable. The two phases in equilibrium are ferrite and austenite between this temperature and **787.13°C**, when ferrite becomes unstable. Austenite is then the only stable phase, and this situation persists up to the liquid solubility temperature of **1453.05°C**. The **BCC_A2** phase known as delta-ferrite is stable in a narrow temperature range at high temperature, and by **1600°C** the only equilibrium phase is **liquid**. There are no changes in phase stability between 600°C and 400°C, as can be seen from the block of lines below **'changing step direction ...'**.

The final three lines of output give the number of steps and total calculation time, the current value of the stepped variable (673.16 K = 400°C) and an **'OK'** message indicating that the calculation was carried out successfully.

The contents of the **'Phase summary'** and **'Phase details'** are not modified during the stepped calculation, but still display the information loaded from the calculation state **'Equil @ 600°C'**.

BUFFERS

All the equilibria listed above are stored in a buffer. In other words, a buffer is a collection of calculation states (in this case, every calculation state was created in a different temperature). The default buffer is named **'_default_'**, and its contents are overwritten when a new stepped calculation is carried out.

To be able to keep more than one set of stepped equilibria, additional buffers must be created. Firstly, rename the existing default buffer using **'Global > Buffers > Rename'**. Type **'T=400 to 1600°C'** into the **'New buffer name'** box and click **'OK'**. Then, create a new buffer using **'Global > Buffers > Create'**. This new buffer will contain the results from a new stepped equilibrium calculation in which the carbon content is varied from 0 to 1.5 wt.% at 500°C, so enter the name 'C=0 to 1.5 at 500°C'. Note that buffers can be selected from the drop-box in the toolbar area or using 'Global > Buffers > Select'.
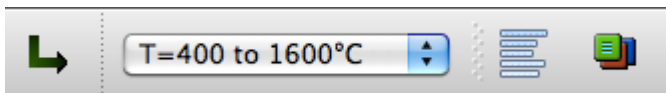
STEPPED EQUILIBRIUM CALCULATION WITH VARYING CARBON CONTENT

RUNNING THE CALCULATION

Calculate an equilibrium at 500°C. Open the **'Step equilibrium'** window again, but this time select **'Element cont..'** instead of **'Temperature'** in the **'Type'** box. Enter **'0'**, **'1.5'** and **'0.05'** respectively as the start, stop and step interval values. (Note that, as shown in the image below, MatCalc accepts either a decimal point or a comma as the decimal separator.) In the **'Boundary conditions'** box, ensure that the element selected is **'C'**, and enter the temperature as **'500'**. Ensure that in the **'vary'** box, **'global comp'** is selected, and that in the **'Options'** column, **'Temperatures in Celsius'** and **'Composition in weight percent'** are both selected, then click on **'Go'**.
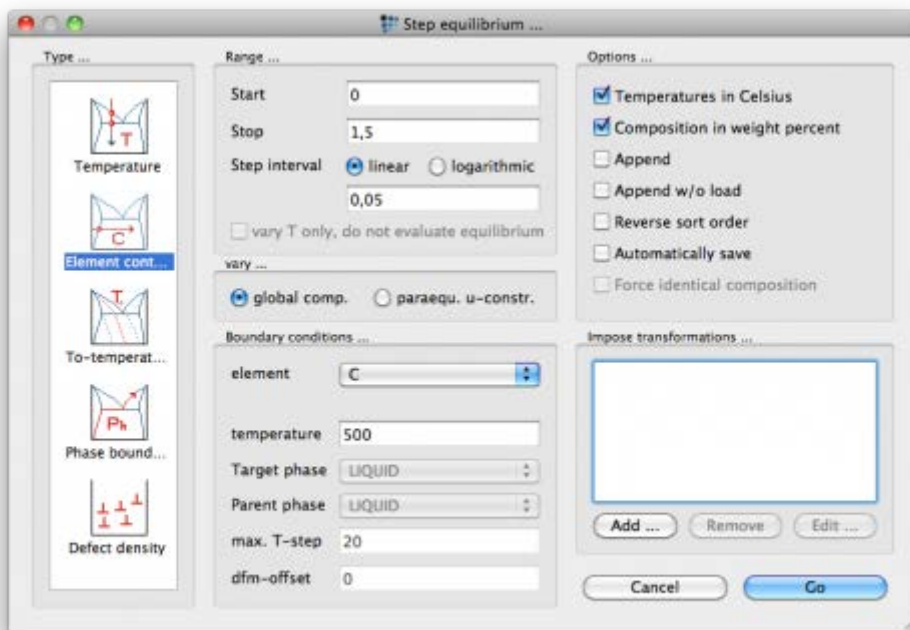
The contents of the **'Output'** window should appear as follows:

```
1, 0.00 s, 0.4, its 2,  BCC_A2 CEMENTITE - OK -
2, 0.00 s, 0.45, its 2,  BCC_A2 CEMENTITE - OK -
3, 0.00 s, 0.5, its 2,  BCC_A2 CEMENTITE - OK -
4, 0.00 s, 0.55, its 2,  BCC_A2 CEMENTITE - OK -
5, 0.00 s, 0.6, its 2,  BCC_A2 CEMENTITE - OK -
6, 0.00 s, 0.65, its 2,  BCC_A2 CEMENTITE - OK -
7, 0.00 s, 0.7, its 2,  BCC_A2 CEMENTITE - OK -
8, 0.00 s, 0.75, its 2,  BCC_A2 CEMENTITE - OK -
9, 0.00 s, 0.8, its 2,  BCC_A2 CEMENTITE - OK -
10, 0.00 s, 0.85, its 2,  BCC_A2 CEMENTITE - OK -
11, 0.00 s, 0.9, its 2,  BCC_A2 CEMENTITE - OK -
12, 0.00 s, 0.95, its 2,  BCC_A2 CEMENTITE - OK -
13, 0.00 s, 1, its 2,  BCC_A2 CEMENTITE - OK -
14, 0.00 s, 1.05, its 2,  BCC_A2 CEMENTITE - OK -
15, 0.00 s, 1.1, its 2,  BCC_A2 CEMENTITE - OK -
16, 0.00 s, 1.15, its 2,  BCC_A2 CEMENTITE - OK -
17, 0.00 s, 1.2, its 2,  BCC_A2 CEMENTITE - OK -
18, 0.00 s, 1.25, its 2,  BCC_A2 CEMENTITE - OK -
19, 0.00 s, 1.3, its 2,  BCC_A2 CEMENTITE - OK -
20, 0.00 s, 1.35, its 2,  BCC_A2 CEMENTITE - OK -
21, 0.00 s, 1.4, its 2,  BCC_A2 CEMENTITE - OK -
22, 0.00 s, 1.45, its 2,  BCC_A2 CEMENTITE - OK -
23, 0.00 s, 1.5, its 2,  BCC_A2 CEMENTITE - OK -
changing step direction ...
24, 0.00 s, 0.35, its 2,  BCC_A2 CEMENTITE - OK -
25, 0.00 s, 0.3, its 2,  BCC_A2 CEMENTITE - OK -
26, 0.00 s, 0.25, its 2,  BCC_A2 CEMENTITE - OK -
27, 0.00 s, 0.2, its 2,  BCC_A2 CEMENTITE - OK -
28, 0.00 s, 0.15, its 2,  BCC_A2 CEMENTITE - OK -
29, 0.00 s, 0.1, its 2,  BCC_A2 CEMENTITE - OK -
30, 0.00 s, 0.05, its 2,  BCC_A2 CEMENTITE - OK -
Xsol 'CEMENTITE': X(C): 5.6263874e-05, WP(C): 0.0012101191 - OK -
31, 0.00 s, 1e-09, its 4,  BCC_A2 - OK -
Steps: 32, CalcTime: 0.62 s
AktStepVal: 0.000000
- OK -
```

Similarly to the temperature-step calculation, the output consists of a series of equilibria evaluated at the specified step-values. The first of these corresponds to the carbon content of 0.4 wt.% entered in the **'System composition'** box in Tutorial 2. The carbon content is then increased in 0.05 wt.% steps up to the maximum value of 1.5 wt.%. The 'Changing step direction' line marks the beginning of the second set of equilibria, in which the carbon content is decreased. At 500°C, the stable phases are BCC_A2 and CEMENTITE across almost the whole composition range, but between the final two equilibria there is a line beginning with **'Xsol'**. The line below this gives the carbon content at which cementite becomes unstable, both in mole fraction **'X(C)'** and in weight percent **'WP(C)'**. Create a third buffer named **'C=0 to 1.5 at 800°C'** and perform a stepped calculation with the same composition range but at a temperature of 800°C. The output in this case includes three **'Xsol'** lines, corresponding to changes in phase stability:

```
1, 0,02 s, 0,4, its 49, FCC_A1 - OK -
2, 0,00 s, 0,45, its 3, FCC_A1 - OK -
3, 0,00 s, 0,5, its 3, FCC_A1 - OK -
4, 0,00 s, 0,55, its 3, FCC_A1 - OK -
5, 0,00 s, 0,6, its 3, FCC_A1 - OK -
6, 0,00 s, 0,65, its 3, FCC_A1 - OK -
7, 0,00 s, 0,7, its 3, FCC_A1 - OK -
8, 0,00 s, 0,75, its 3, FCC_A1 - OK -
9, 0,00 s, 0,8, its 3, FCC_A1 - OK -
10, 0,02 s, 0,85, its 3, FCC_A1 - OK -
11, 0,00 s, 0,9, its 3, FCC_A1 - OK -
Xsol 'CEMENTITE': X(C): 0.042626921, WP(C): 0.94851252 - OK -
12, 0,01 s, 0,95, its 4, FCC_A1 CEMENTITE - OK -
13, 0,00 s, 1, its 2, FCC_A1 CEMENTITE - OK -
14, 0,00 s, 1,05, its 2, FCC_A1 CEMENTITE - OK -
15, 0,00 s, 1,1, its 2, FCC_A1 CEMENTITE - OK -
16, 0,00 s, 1,15, its 2, FCC_A1 CEMENTITE - OK -
17, 0,00 s, 1,2, its 2, FCC_A1 CEMENTITE - OK -
18, 0,00 s, 1,25, its 2, FCC_A1 CEMENTITE - OK -
19, 0,00 s, 1,3, its 2, FCC_A1 CEMENTITE - OK -
20, 0,00 s, 1,35, its 2, FCC_A1 CEMENTITE - OK -
21, 0,00 s, 1,4, its 2, FCC_A1 CEMENTITE - OK -
22, 0,00 s, 1,45, its 2, FCC_A1 CEMENTITE - OK -
23, 0,00 s, 1,5, its 2, FCC_A1 CEMENTITE - OK -
changing step direction ...
24, 0,00 s, 0,35, its 4, FCC_A1 - OK -
Xsol 'BCC_A2': X(C): 0.015673104, WP(C): 0.34127957 - OK -
25, 0,02 s, 0,3, its 4, FCC_A1 BCC_A2 - OK -
26, 0,00 s, 0,25, its 2, FCC_A1 BCC_A2 - OK -
27, 0,00 s, 0,2, its 2, FCC_A1 BCC_A2 - OK -
28, 0,00 s, 0,15, its 2, FCC_A1 BCC_A2 - OK -
29, 0,00 s, 0,1, its 2, FCC_A1 BCC_A2 - OK -
30, 0,00 s, 0,05, its 2, FCC_A1 BCC_A2 - OK -
Xsol 'FCC_A1': X(C): 0.000555891, WP(C): 0.011960753 - OK -
31, 0,01 s, 1e-009, its 9, BCC_A2 - OK -
Steps: 32, CalcTime: 0,30 s
AktStepVal: 0,000000
- OK -
```

EDIT BUFFER STATES

The **'Output'** window provides information on which phases are stable at a given temperature and carbon content, but not on the phase fractions or compositions. However, this detailed information is stored in the buffers and can be found by selecting **'Global > Buffers > Edit buffer states'**.
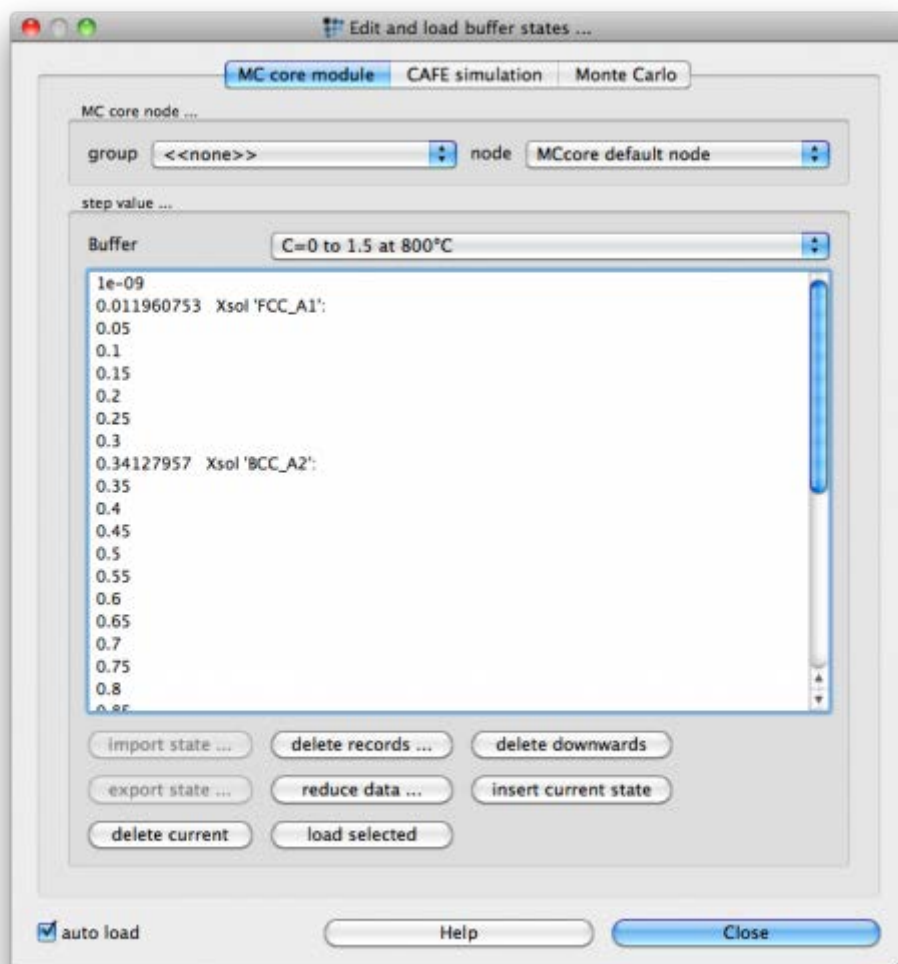
The upper part of this window contains a drop-box for selecting a buffer, and the lower part gives a list of the step-values at which equilibria have been evaluated. These are either temperature or carbon content values, depending on the buffer chosen, and their units are those specified in the **'Step equilibrium'** window when setting up the calculation. The **'Tsol'** or **'Xsol'** values are also stored. If the **'auto load'** box at the bottom left is ticked, clicking on a step-value loads the equilibrium, and the contents of the **'Phase summary'** and **'Phase details'** are immediately updated with phase fraction and composition details for this equilibrium. The next two tutorials demonstrate how to produce graphical plots of phase fractions, compositions and many other quantities as a function of the stepped variable.

TO FINISH…

Save the workspace file - it will be needed again in Tutorial 4.

CONSECUTIVE ARTICLES

The tutorial is continued in article T4 - Graphical presentation and export of results

T4: GRAPHICAL PRESENTATION AND EXPORT OF RESULTS

This tutorial was tested on
MatCalc version 5.50 rel 0.057
*license: free*
database: mc_sample_fe.tdb

CONTENTS

- Creating a new graphical window
- Introduction to the variables window
- Modifying the appearance of a plot using 'options'
- Zooming in and displaying x- and y-values
- Exporting a plot as an image and as numerical data

BEFORE STARTING…

Open the file saved from Tutorial 3 and select the buffer named **'T=400 to 1600°C'**.

PLOTTING A GRAPH

To plot numerical results, it is first necessary to create a graphical window. In the **'View'** menu, click on **'Create new window'** or click on icon.
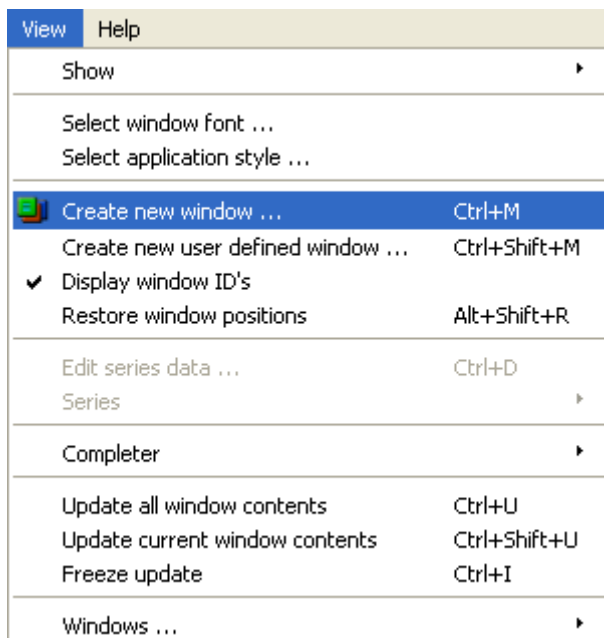
In the **'Create new window'** box which appears, there is a list of a number of possible window types. Among these are **'(a1)'**, **'(a5)'** and **'(a6)'**, which are the familiar **'output'**, **'phase summary'** and **'phase details'** windows automatically placed on the screen when a new workspace file is created.

Select type **'(p1) Plot: XY-data'** and click on **'OK'**
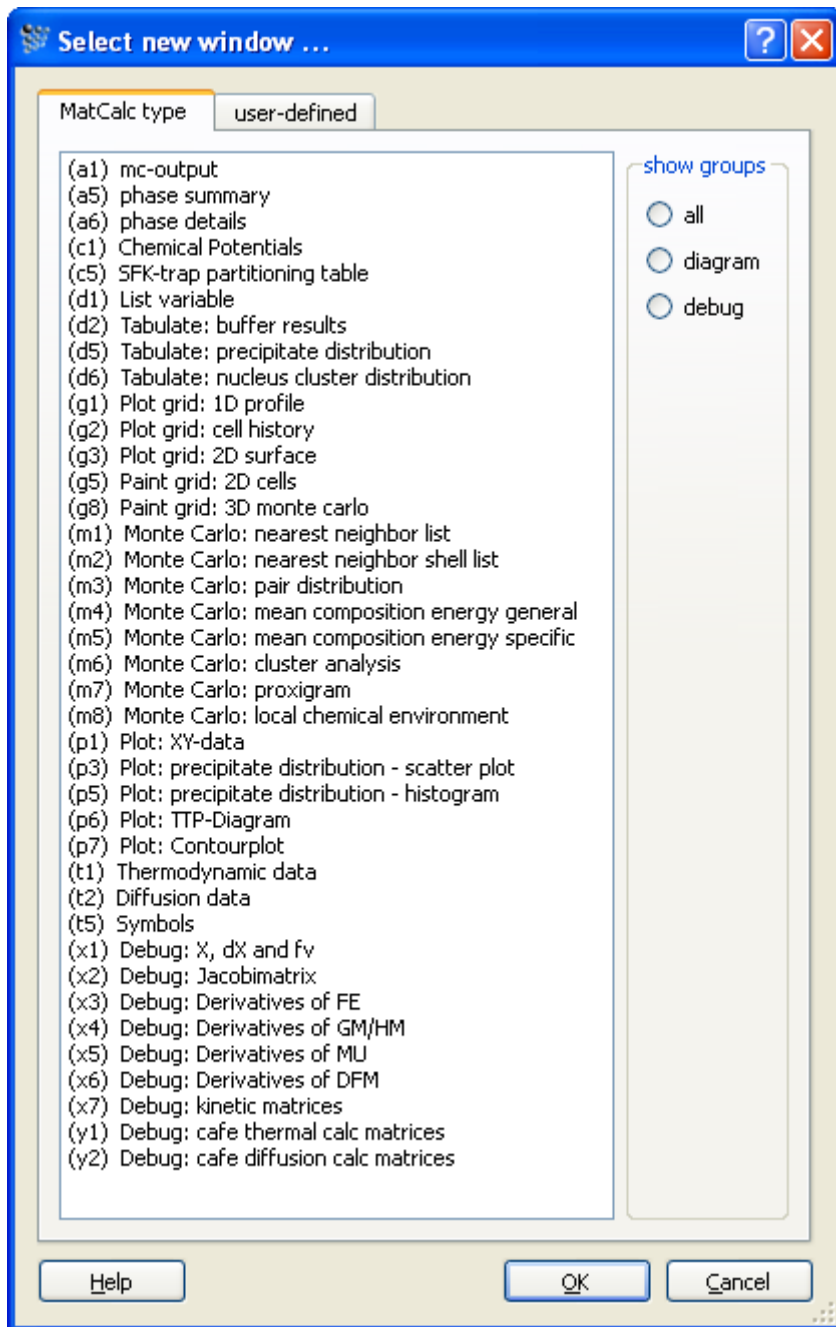
An empty plot with x- and y-axes appears on the screen. Locate the **'Variables'** window. (If it is not present, right-click in the toolbar area at the top of the screen and select it from the menu, or click on **'Show variables window'** in the **'View'** > **'Show'** submenu.) Expand the **'favorites'** section by clicking on the small plus-sign to its left. Then, further expand the section labelled **'F$*'** to give the list shown below.
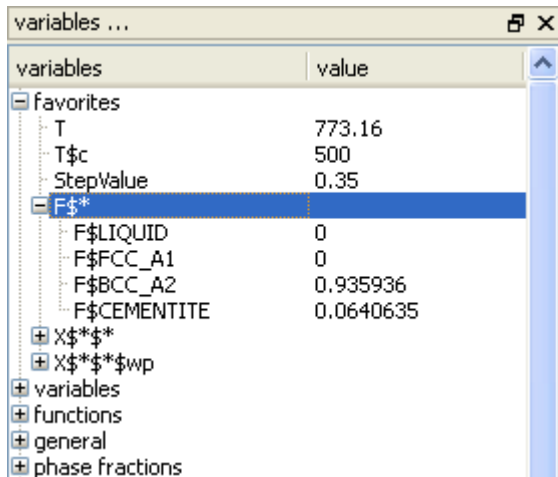
The syntax **'F$BCC_A2'** means **'the phase fraction of BCC_A2'**, where the dollar sign is a separator between the variable **'F'** and the phase to which it applies **'BCC_A2'**. In the heading of the list, **'F$*'**, the asterisk is a wild-card indicating **'all phases'**. Select **'F$*'**, drag it to the empty plot and drop it.

The plot should appear as shown below:
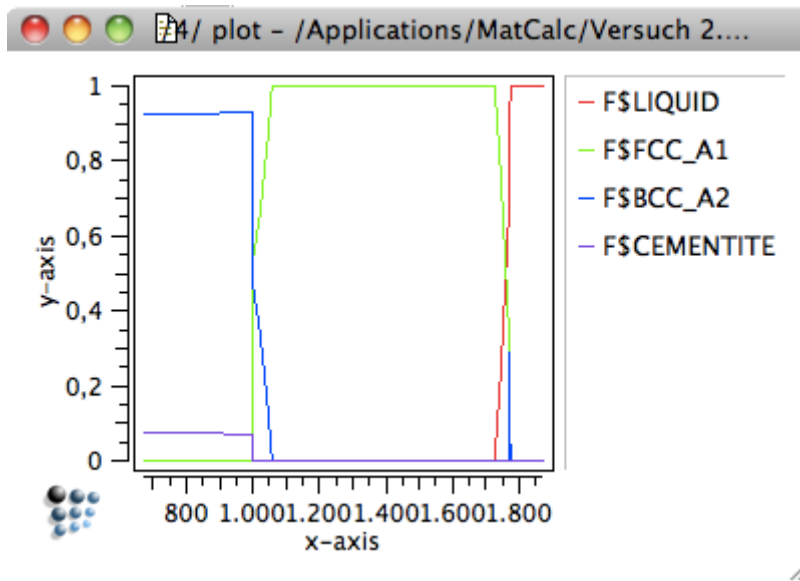
CHANGING THE APPEARANCE OF THE PLOT

RESULTS FROM DIFFERENT BUFFERS

The **'Options'** window can now be used to modify the appearance of the plot as required. (Again, if this is not currently shown, it can be made to appear using the View menu or the right-click menu in the toolbar area.)
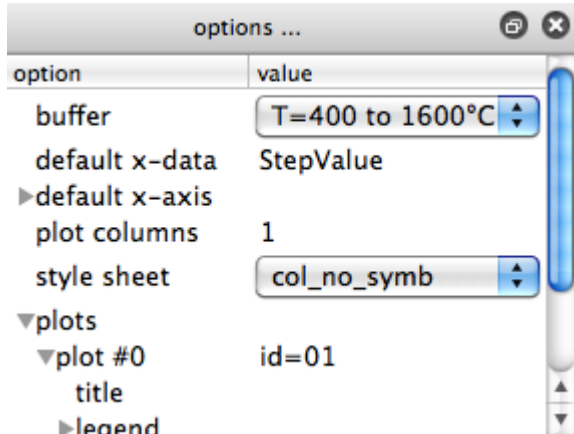
Firstly, note that there is a **'buffer'** drop-box. By selecting one of the other buffers, the contents of the plot can be changed. The **'default x-data'** option (the second line down in the options window) is set to StepValue, i.e. the value of the stepped variable used in the stepped equilibrium calculation.

Thus, on selecting the **'C=0 to 1.5 at 500°C'** buffer, the x-value changes to carbon content, and the plot looks like this:
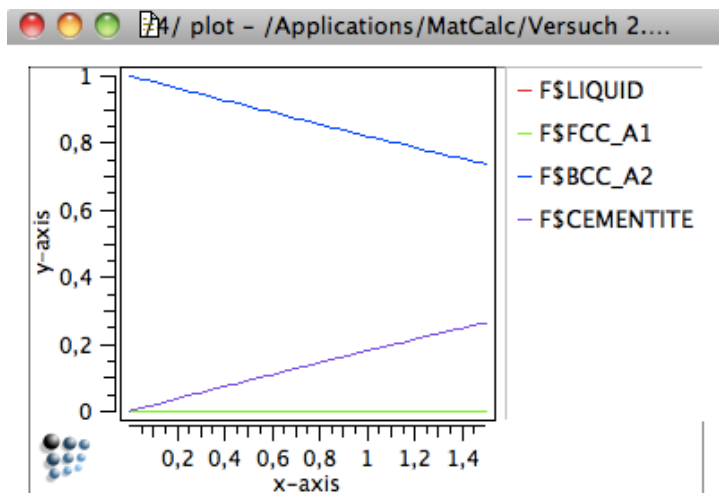

and the plot for the **'C=0 to 1.5 at 800°C'** buffer looks like this:
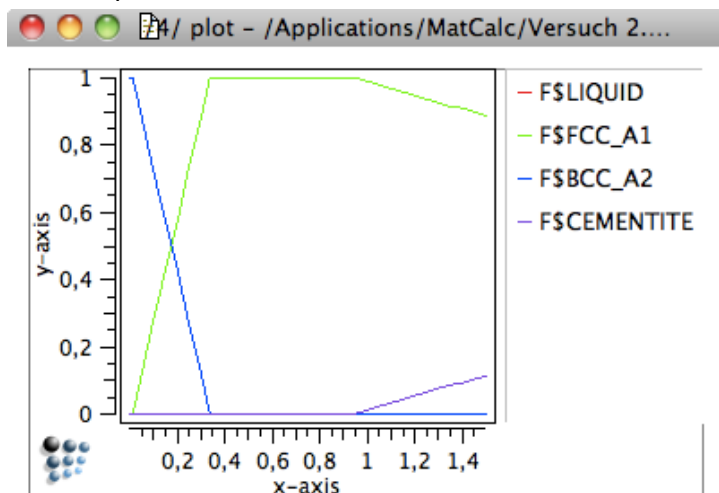
Select the **'T=400 to 1600°C'** buffer from the buffer drop-box. One of the first things to note is that the x-axis data does not run from 400 to 1600; this is because the step value is expressed by default in Kelvin rather than in Celsius. To change this, double-click on the **'default x-data'** line. A box appears, entitled **'New value for 'default x-data''**. Enter **'T$C'** (temperature in Celsius) in place of **'StepValue'**.
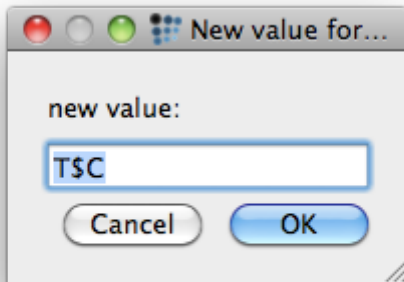
The plot can be changed from colour to black-and-white (**'b/w'**) using the **'style sheet'** drop box.

The **'plots'** section of the options menu can be expanded using the plus-sign. Below **'plot#0'** (the name of the current plot) is a list of options for this plot:
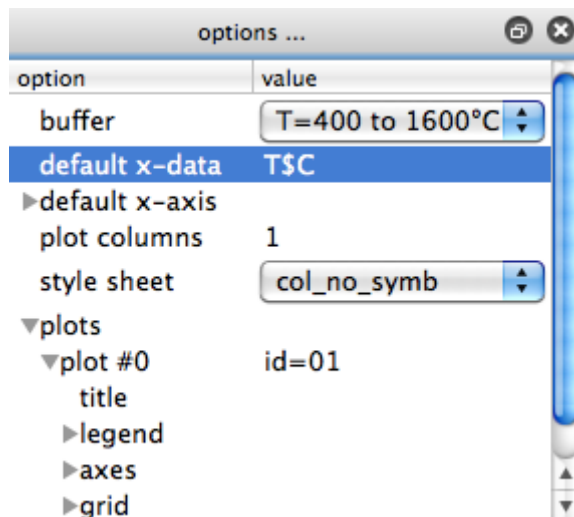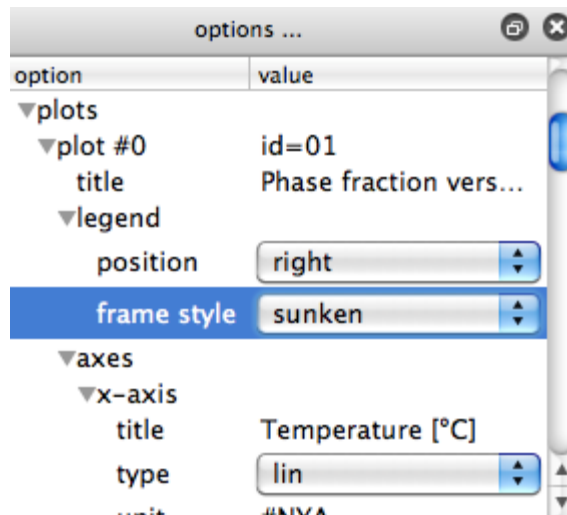
TITLE

This is blank by default. Double-click to enter a title, e.g. **'Phase fraction versus temperature for Fe-0.4 wt.%C'**.
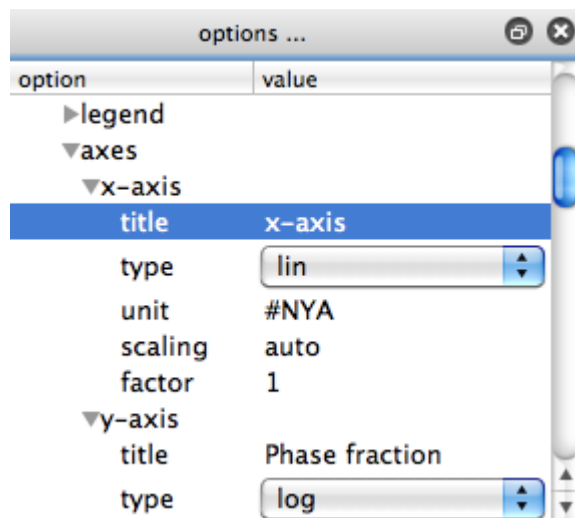
LEGEND

This comprises options for the position of the legend and for the style of the box surrounding it.
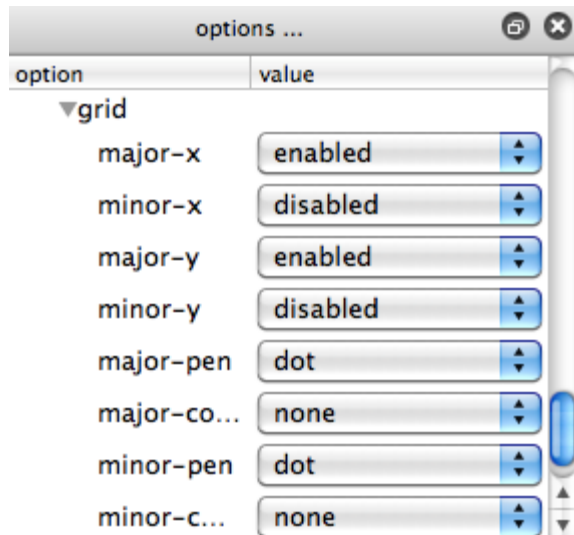

AXES

The 'axes' section expands to give options for the **'x-axis'**, **'y-axis'**, **'2nd x-axis'** and **'2nd y-axis'** (the latter two are not used in the current plot).

Double-clicking on the **'title'** line will bring up a box entitled **'New value for title'**. Enter **'Temperature [°C]'**. In the same way, change the y-axis title to **'Phase fraction'**. The axis type can be set to either linear or logarithmic. A linear scale is more suitable for the temperature axis, but a logarithmic y-axis enables the fractions of minor phases, such as cementite in this example, to be seen more clearly. Change **'lin'** to **'log'** for the y-axis. The automatically assigned minimum y-value on the log-scale may not be appropriate, so if this is the case, double-click on **'scaling'** and replace **'auto'** with **'0.01..1'**. The two numbers are the lower and upper limits respectively. If one or other of these is missed off, an automatic value is assigned instead. (For example, using **'0.01..'** is sufficient to give a scale from 0.01 to 1, since 1 is the maximum value of F$*).

GRID

This allows gridlines to be added to the plot, and their appearance to be modified. Change **'disabled'** to **'enabled'** for **'major-x'** and **'major-y'** to show major gridlines.

option	value
▼grid	
major-x	enabled
minor-x	disabled
major-y	enabled
minor-y	disabled
major-pen	dot
major-co...	none
minor-pen	dot
minor-c...	none

SERIES

Expanding the **'series'** section gives a list of options for each data-series. The name of the series (as it appears in the legend) can be changed using **'name'**.

The **'locked'** option, when set to **'yes'**, protects the series from any changes when the contents of the buffer are updated. A locked series is indicated by an asterisk by the name, if the automatic name is used.

**'Derivative'** can be used to display the numerically evaluated first or second derivative of a series.

The **'x-data'** and **'y-data'** options control which data-sets are displayed on the x- and y-axes. If the **'x-data'** is set to **'auto'**, the default x-data, as specified above, is used.

The appearance of the plots can be modified by setting **'default style'** to **'no'** rather than **'yes'**, and then expanding **'line'** and **'marker'** to give a list of options for colours, styles, sizes etc.

The image below gives an example of a modified plot.
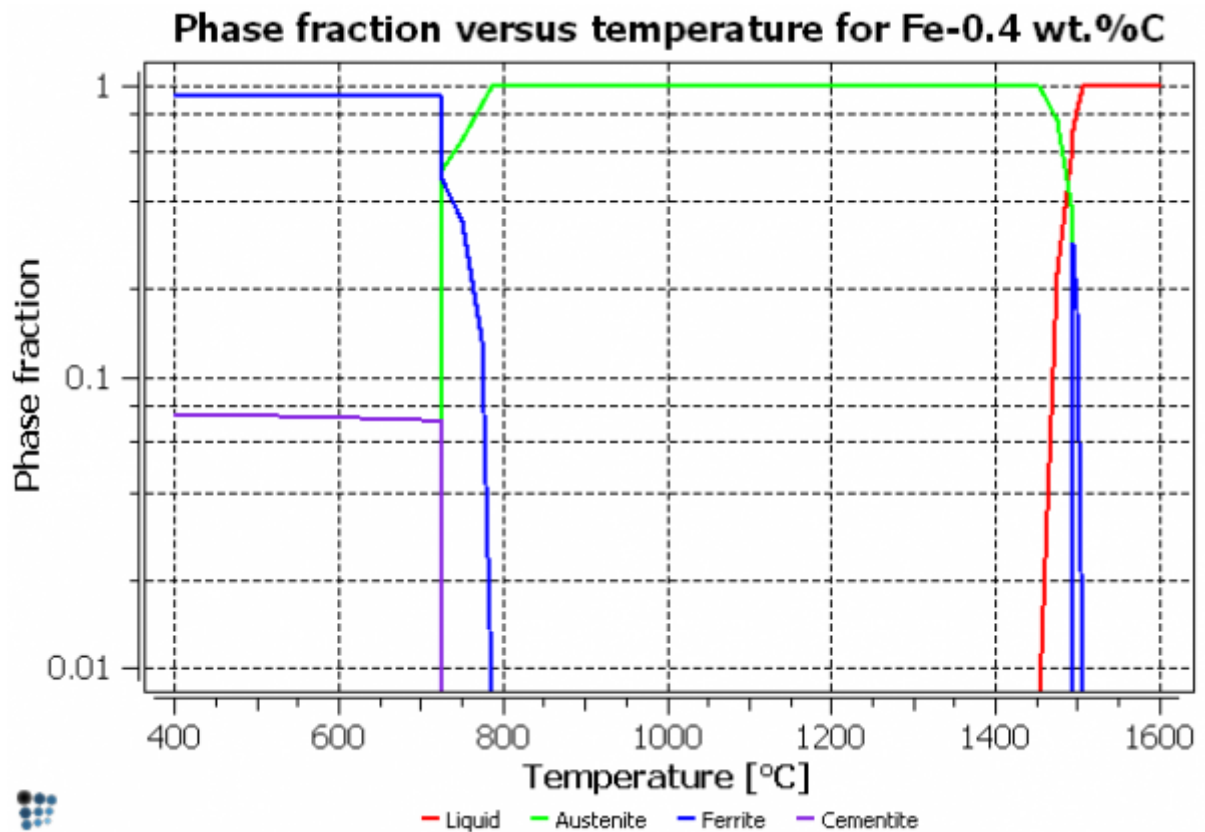
OTHER PLOT OPERATIONS

ZOOMING AREAS OF THE PLOT

Left-click in the plot area and drag the mouse to draw a rectangular box. When the mouse button is released, an enlarged version of the region within the box is shown on the axes. Right-click anywhere in the plot area to return to the original scale.

DISPLAYING X- AND Y-VALUES

When moving the mouse pointer on the plot area, a black cross appears with the y- and x-values next to it. The coordinates of the centre of the cross are also shown on the **status bar** at the **bottom left of the screen**. A larger, red cross can be obtained by pressing the right mouse button.

EXPORTING DATA FROM THE PLOT

Right-clicking in the plot window but outside the area of the plot itself gives a context menu as shown below.
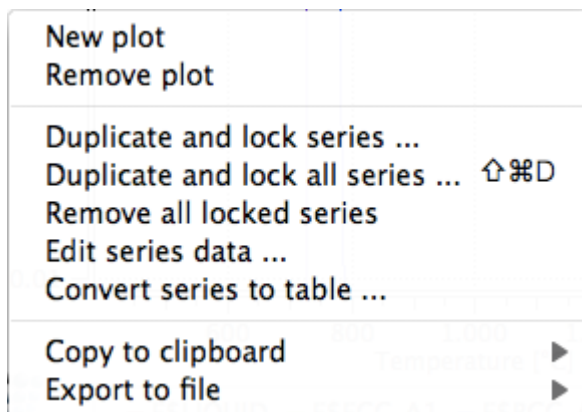
Clicking on **'Copy to clipboard'** allows to export the plot or the frame (which is a plot with some blank space around it) in the **pixmap** (.bmp) or scalar vector graphics (**.svg**) format. Then the exported piece can be pasted to the relevant graphical application. Additional for the plot, there is a possibility to export the numerical **data** which will appear in the form of tab-separated columns after the paste operation.

Clicking on the **'Export to file'** will create the file containing the plot with or without the frame. The possible output file formats are **'.png'**, **'.svg'** and **'.pdf'**

TO FINISH...

Save the workspace file.

CONSECUTIVE ARTICLES

The tutorial is continued in article T5 - MatCalc built-in variables; graphical output

T5: MATCALC BUILT-IN VARIABLES; GRAPHICAL OUTPUT

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb

CONTENTS

- Adding further plots to a plot window
- Using the built-in variables
- Defining a default x-axis
- Modifying the series
- Adding a new series to a plot
- Removing a series from a plot
- Duplicating and locking series
- Editing series data
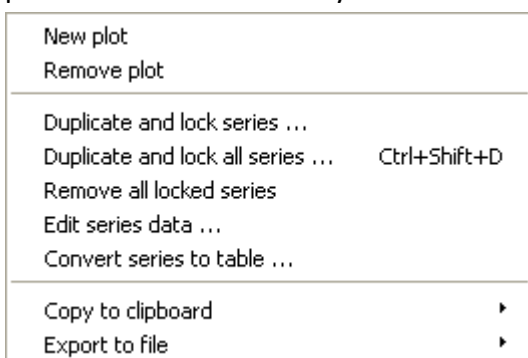- Converting series to tables

BEFORE STARTING…

Re-open the file saved in Tutorial 4 and save it under a new name.

ADDING PLOTS OF DIFFERENT VARIABLES

CREATING A NEW PLOT

Highlight the plot window and right-click in this window outside the plot area to bring up the plot context menu already seen in Tutorial 4. Click on **'New plot'**.


An empty plot appears below the original one.

VARIABLES

As well as the phase fraction variables **'F$*'** encountered in the previous tutorial, MatCalc contains many other built-in variables which are evaluated at each step-value of the stepped equilibrium calculations. These can be found in the variables window. Information about each variable is contained in the small window below the main variables window. Locate the **'driving forces'** category and drag **'DFM$*'** to the empty plot window, to give a plot as shown below.
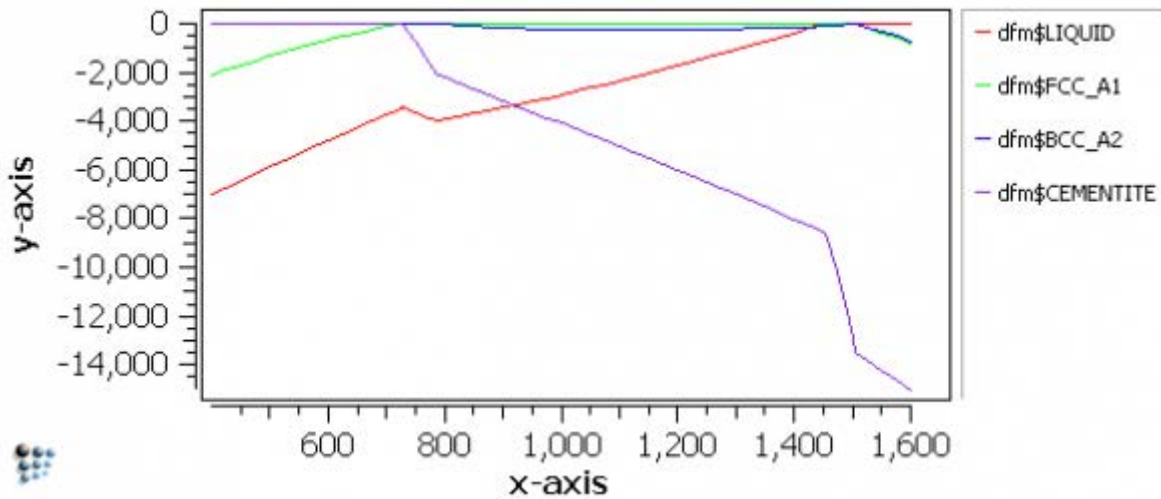
Other variable categories of particular interest for stepped equilibrium calculations are highlighted in blue in the image below:
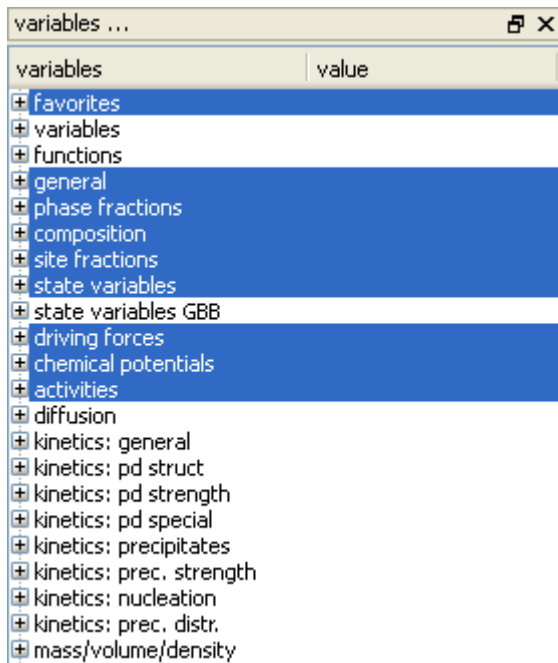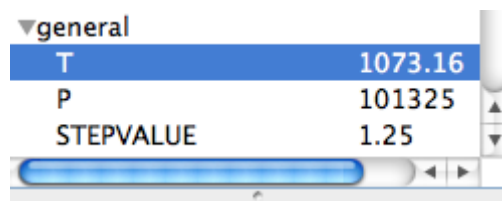
- 'FAVORITES'

This contains the most frequently needed variables: temperature in Kelvin ('**T**') and in Celsius ('**T$C**'), step-value, phase fractions ('**F$***') and compositions expressed in mole fraction ('**X$*$***') and in weight percent ('**X$*$*$wp**'). In these composition variables, the first asterisk represents the phase, and the second, the element, for example '**X$LIQUID$C**'.

-'GENERAL'

Temperature, step-value and pressure can also be found under this category. The temperature is in Kelvin by default, but the temperature in Celsius can be obtained by appending '**$C**', as has already been seen in the '**Favorites**' category. This suffix is known as a '**unit qualifier**'. The '**information on variables**' window shows the valid unit qualifiers for the variables:


```
▼general
    T              1073.16
    P              101325
    STEPVALUE      1.25

category: general
expression: T
legal unit qualifiers: c
-> temperature
```

- 'PHASE FRACTIONS'

The phase fractions '**F$***' are repeated here.

- 'COMPOSITION'

This contains the '**X$*$***' composition variables mentioned above, and a number of other composition-related variables, expressed either as either **mole fractions (X…)** or as **u-fractions (U…)**. (Not all of these are applicable to stepped-equilibrium calculations, however: '**XP$*$***' and '**UP$*$***' are for precipitation calculations.)

Compositions in weight percent are not given separately here, but it can be seen from the '**variables information**' window that '**wp**' is a valid unit qualifier for the variables beginning with '**X**'. This means that weight percentages can be obtained by appending '**$wp**' to the names of these variables.

- 'SITE FRACTIONS'

The '**Y$*$*$***' variables give the site fraction of an element on a particular sublattice of a phase. For example, BCC_A2 has the variables '**YBCC_A2FE$0**' (site fraction of iron on sublattice 0) and '**YBCC_A2C$1**' (site fractions of carbon and vacancies on sublattice 1). The '**YX$*$***' variables represent the mole fraction of an element on a particular sublattice position of a phase; in this case, vacancies are not considered.

- 'STATE VARIABLES'

This category consists of a number of thermodynamic variables, including molar Gibbs free energies, entropies, enthalpies and heat capacities of the system and of each phase.

**- 'CHEMICAL POTENTIALS', 'ACTIVITIES'**

These categories include chemical potentials **'MU$*$*'**, activities **'AC$*$*'** and activity coefficients **'ACC$*$*'**.

Further plots can be added to the same plot window using **'New plot'**; they will share the same buffer, default x-data and colour scheme. Some examples are shown below:
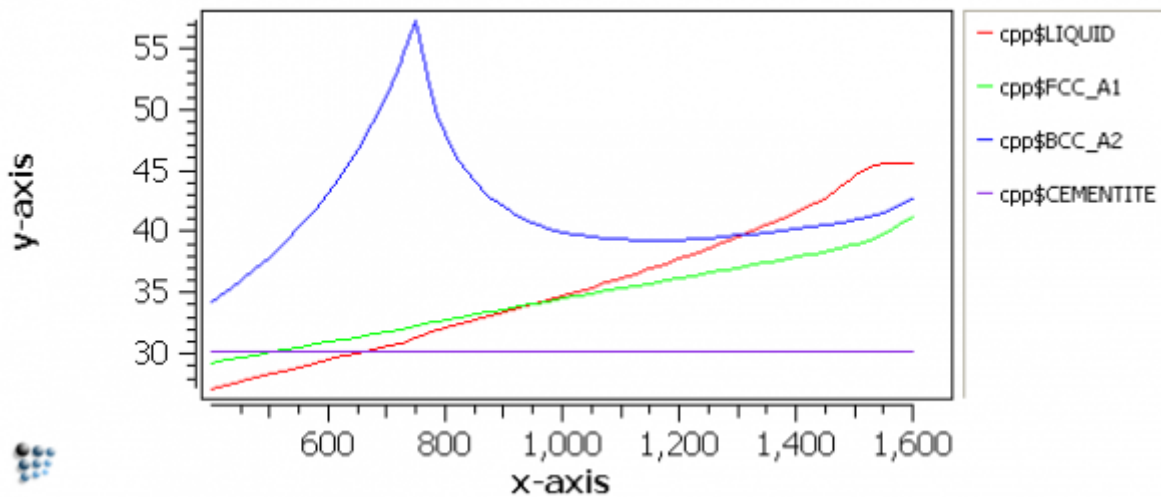
- Molar Gibbs free energy (**'GMP$*'**)
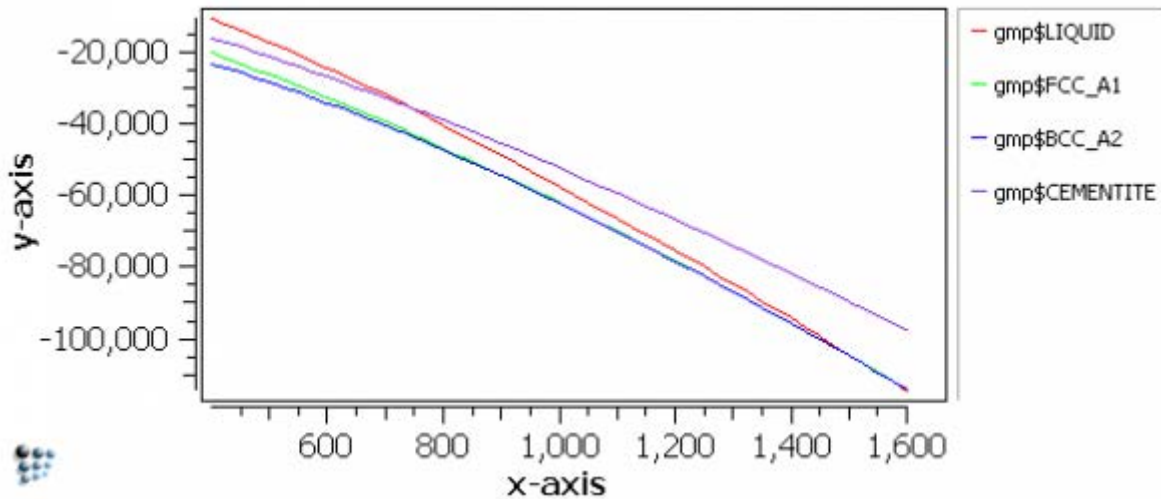
- Chemical potential of carbon (**'MUP$*$C'**) - here, the chemical potential of carbon in the cementite phase was omitted (the scale of y-axis is limited to +10.000)
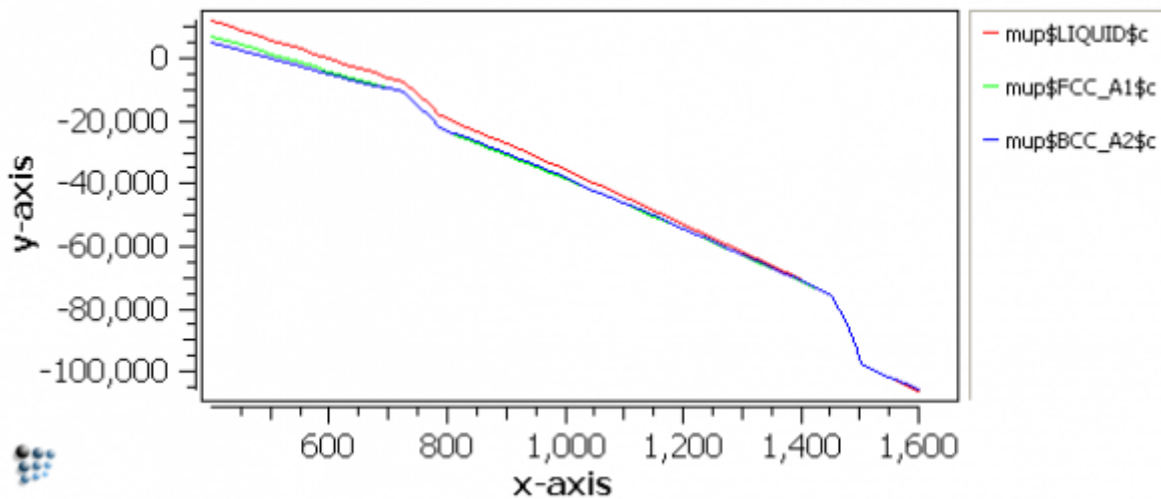

- Molar heat capacity (**'CPP$*'**, note the lambda-anomaly at the Curie temperature in BCC_A2)

ARRANGING PLOTS IN THE COLUMNS

When there are many plots in the plot window then they will get streched so much that they will eventually become unreadable. In order to obtain a transparency, it might be a good idea to arrange the plots in more than one column. To place the plots in two columns, click on **'plot columns'** in **'Options'** window and type **'2'** in the appearing dialog.
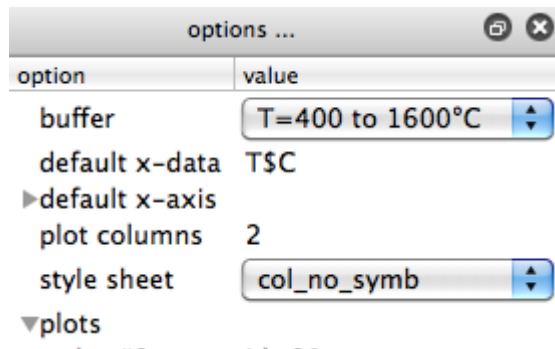

DEFAULT X-AXIS

To give a consistent appearance to all the x-axes in the plot window, a **'default x-axis'** can be defined. This is found towards the top of the **'Options'** window. Change **'no'** to **'yes'** in the 'use for all plots' line and define the properties of the x-axis in the same way as for a normal x-axis.
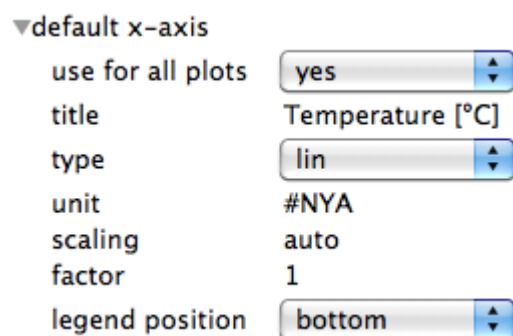
DISPLAYING X-VALUES OF MULTIPLE PLOTS

If the plot window contains several plots, right-clicking and dragging the mouse in one of these will display not only a cross in that plot, but a vertical line at the same x-value in all the others. An example is shown below:
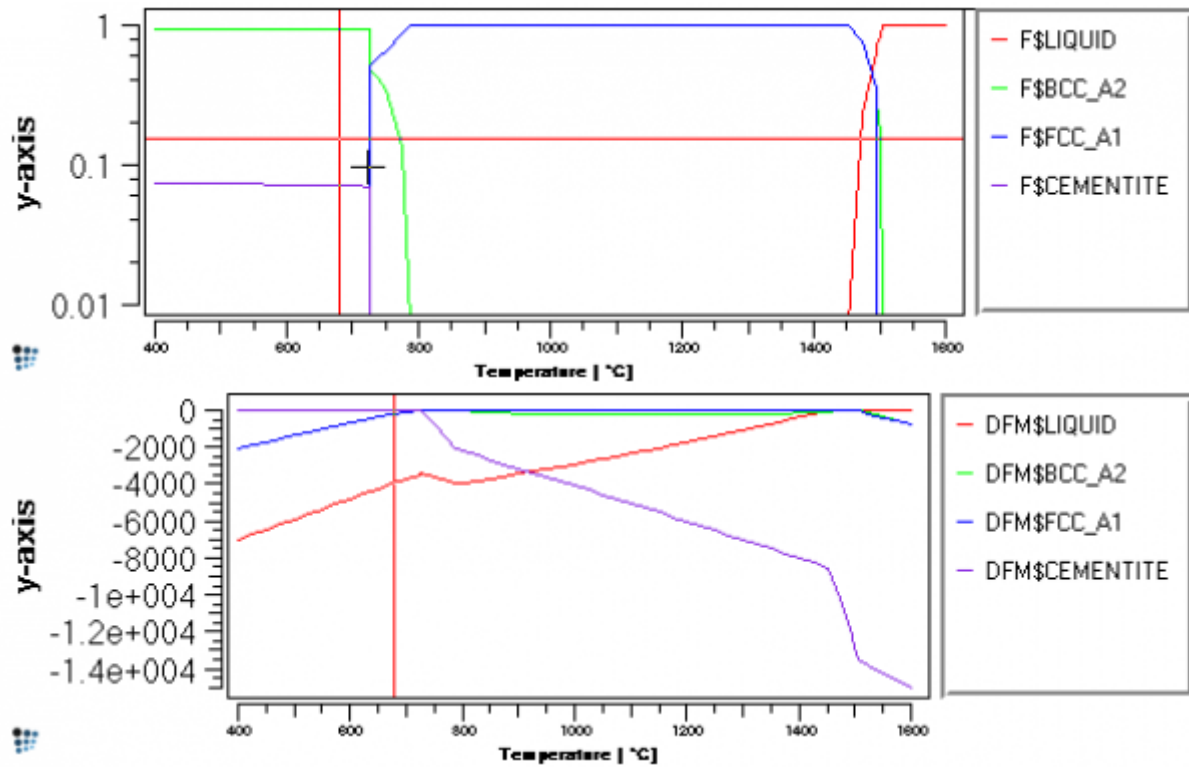

MODIFYING THE SERIES IN A PLOT

This part of the tutorial will demonstrate how to use the unit qualifiers mentioned above. Add a new plot to the plot window and drag and drop **'X$*$C'** (carbon content of the phases) from the **'variables'** window. The resulting plot should look like this:
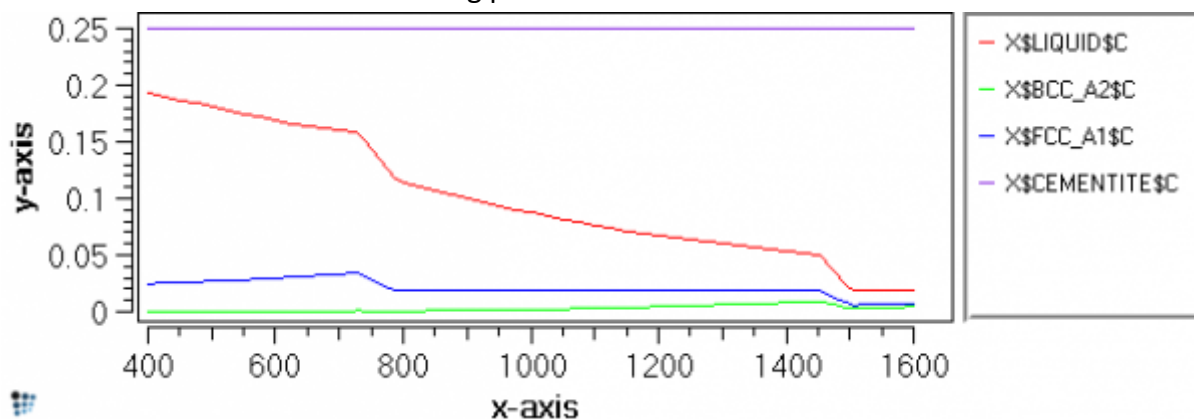
By default, the carbon content is expressed in mole fraction. To change the units to weight percent, firstly click on the new plot to select it. This should expand the section of the **'Options'** list which applies to the new plot. Click on the plus-sign by **'series'** to open the series options:
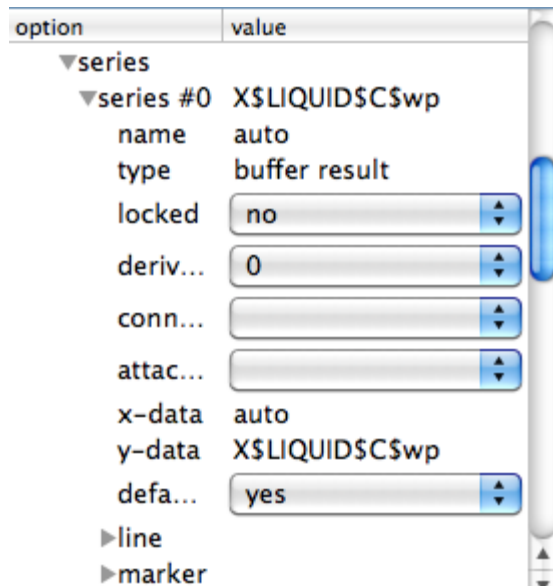
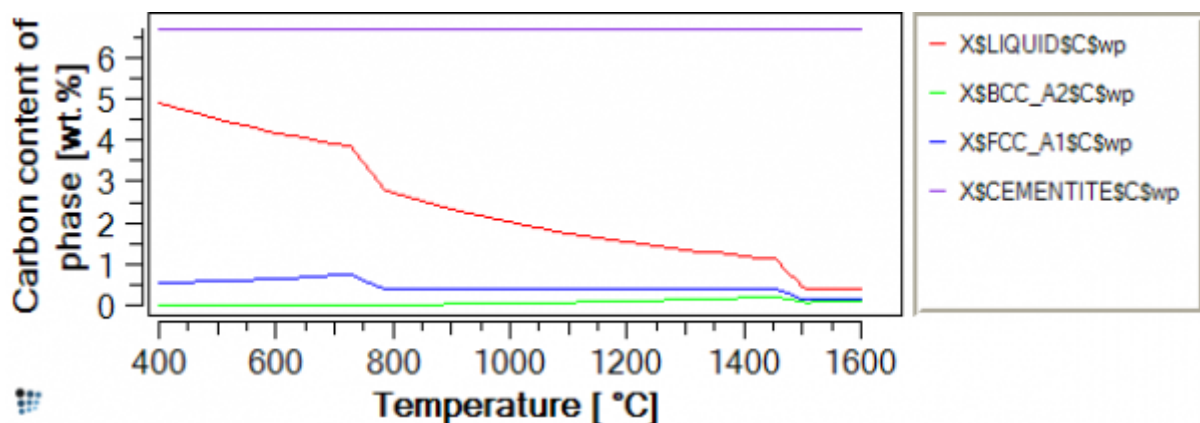Double-click on **'y-data'** for the first series to open the following box. Append **'$wp'** to the existing expression and click **'OK'**.
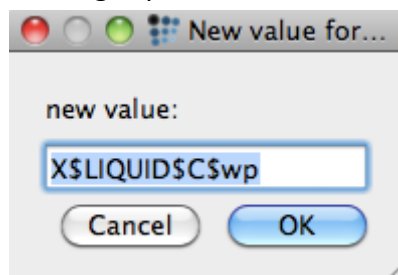
This will change the values plotted for the **'LIQUID'** series. Repeat for the other three series. The final appearance of the plot, with appropriate axis labels added, should be as shown below.

MODIFYING THE SERIES WITH DRAG AND DROP

Alternatively you can select the variable and drag it to the window, and press Ctrl **before** dropping it to the plot. An option window will pop up, where you can modify the original expression (read as %s) by adding mathematical operations or **change** it **to weight percent** by **appending $wp**.
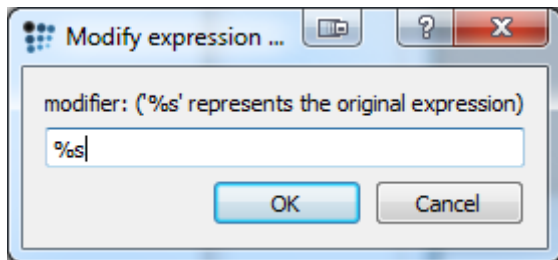
Note: Pressing Ctrl **before** selecting and dragging the desired variable will result in a de-selection. *MatCalc* will hence block you from dropping the variable to a plot, as **nothing** has been selected in reality and an error would occur.
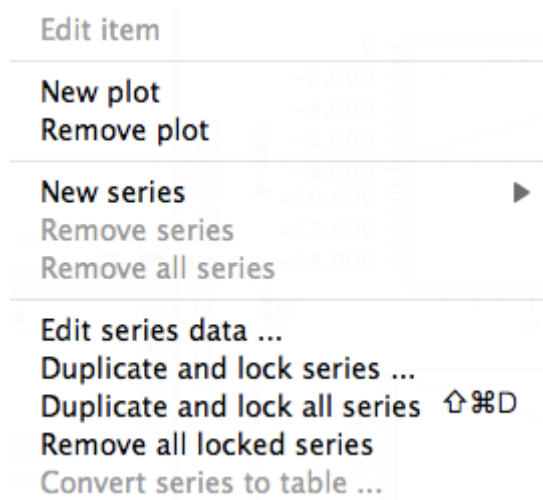
OTHER SERIES OPERATIONS

Right-clicking in the '**Options**' window displays a context menu:

- 'NEW SERIES'

The '**New series**' part of the menu expands to give the following sub-menu.
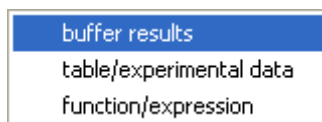
Clicking on '**Buffer results**' creates an empty series (given the name of '**auto**' on the plot) to contain variables evaluated from the results of a buffer. Edit the '**y-data**' line in the '**Options**' window for this series to enter any valid built-in or user-defined variable or an expression. Variables can be copied from the '**Variables**' window by right-clicking on the expression required to display a menu containing Copy, Paste and other operations.
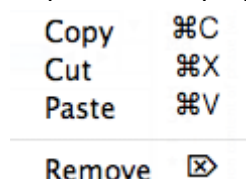
The other series types which can be added are as follows:

'**Table/experimental data**': allows the user to add a set of experimental data points to a plot.

'**Function/expression**': enables an algebraic expression in (x) to be entered.

- 'Remove series', 'Remove all series', 'Remove all locked series'

To remove a series from a plot, first click on the plot to select it. This will expand the part of the Options list which applies to the plot. Select the name of the series from this list and choose **'Remove series'** from the right-click menu (shown above) or press **'Delete'**. Multiple series in the same plot can be selected at once by holding down the CTRL key while clicking on the series names. **'Remove all series'** in the right-click menu deletes all the series in the selected plot. **'Remove all locked series'** removes all the series which are locked (locking the series is described below).

- 'Duplicate and lock series ...', 'Duplicate and lock all series'

This feature is available in the right-click menus of both the Options window and the plot window. Select a series from the list shown and click on **'Duplicate and lock series'**. This will lock the original series and create a copy. **'Duplicate and lock all series'** performs this for all series in the selected plot.

The locked series is protected from any changes when the buffer contents are updated with new calculation results, but the copy is unlocked. This enables easy comparison between results obtained under different conditions.
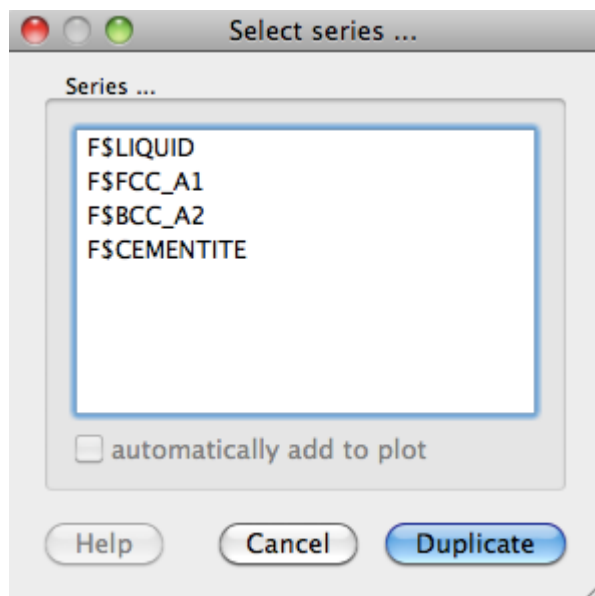
- 'Edit series data ...'

This is also available in both the Options and the plot windows. Select a series and click on **'Edit…'** to display a table containing the numerical data used to plot the graph.
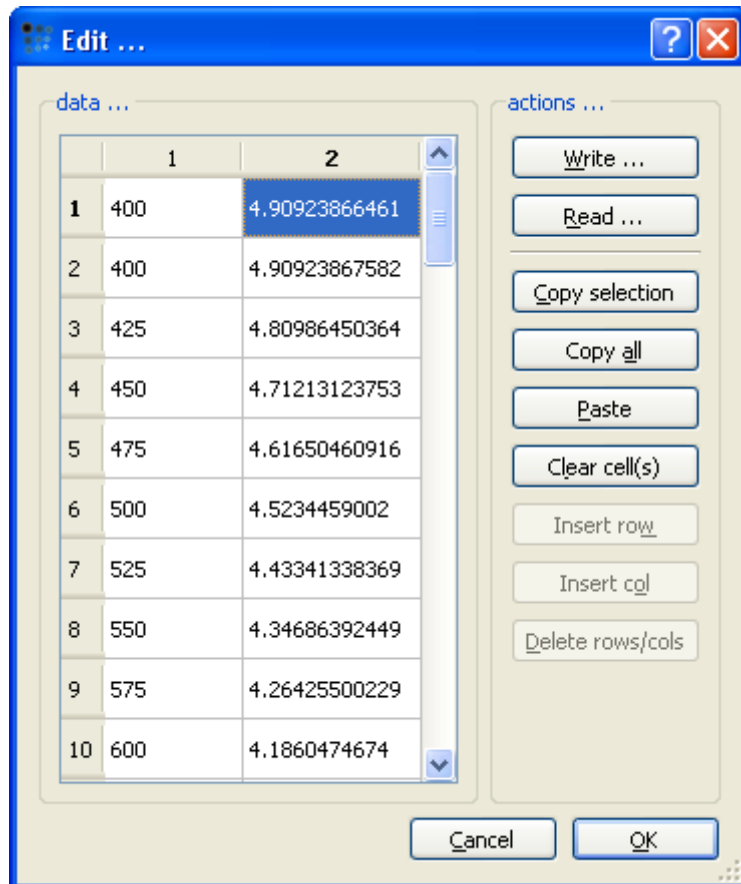
The data can be copied using the **'Copy selection'** or **'Copy all'** buttons. The contents of the rows and columns can be modified using **'Paste'** (to add data copied from another source), **'Clear cell(s)'**, **'Insert row'**, **'Insert col'** and **'Delete rows/cols'** buttons. Use **'Write'** to save the whole dataset to a text file and **'Read'** to load a dataset from a text file.

- **'CONVERT SERIES TO TABLE'**

This places the data from the series into a named table, which can be accessed from the **'Global'** menu.

Select the series, click on **'Convert series to table'**, select the series name and edit the name of the table, if necessary, in the box which appears, as shown below.
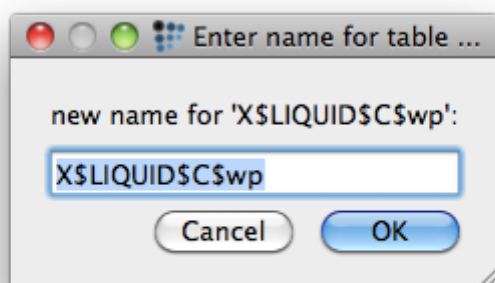
To open and edit a table, select **'Tables and arrays'** from the **'Global'** menu. This will display a list of all the available tables, which can be edited in the same way as the series data described above.
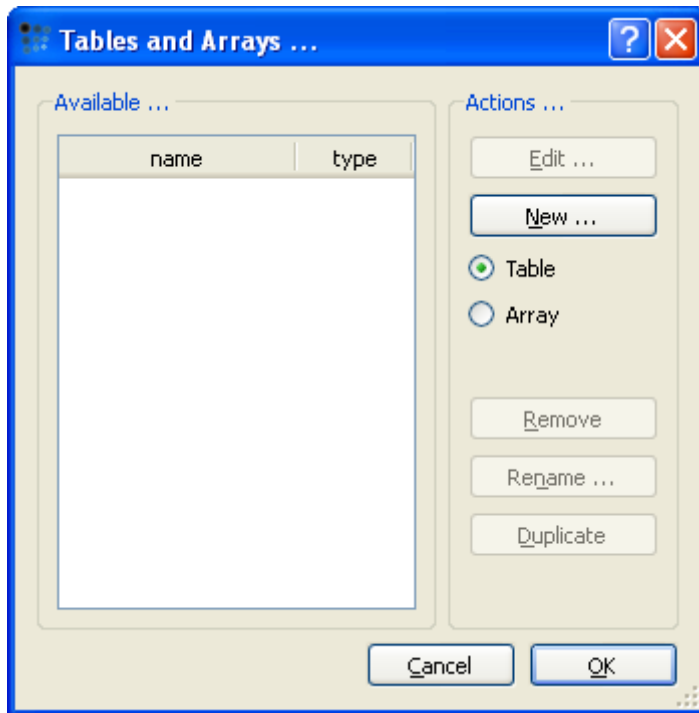
CONSECUTIVE ARTICLES

The tutorial is continued in article T6 - Introduction to user-defined functions.

T6: INTRODUCTION TO USER-DEFINED FUNCTIONS AND VARIABLES

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb

CONTENTS

- Expressions using built-in variables
- Creating a new function
- Using functions
- Defining and using variables

SETTING UP THE SYSTEM

Define a system containing the elements Fe and C and and phases **LIQUID**, **FCC_A1**, **BCC_A2** and **CEMENTITE**. Enter the composition **0.1 wt.% C**. Make a stepped equilibrium calculation, varying the temperature from 400 to 1600°C in 25-degree intervals.

Create a new plot window and drag and drop **'F$*'** from the **'Variables'** window into the plot. Create a second plot in the same window. Set the **'default x-data'** in the Options window to **'T$C'**, and define a default x-axis for all plots labelled **'Temperature [°C]'**.

COMBINING BUILT-IN VARIABLES IN NEW EXPRESSIONS

In systems consisting of a matrix and carbides, it may be interesting to determine how much of the carbon in the system is present in the form of carbides, and how much remains in the matrix phase(s), at any given temperature.

The phase fraction **'F$*'** represents the number of moles of phase per mole of system, and the carbon content of a phase **'X$*$C'** represents the number of moles of carbon per mole of phase. The product of these quantities for a given phase gives the number of moles of carbon in the phase.

To plot this, first drag **'X$*$C'** to the new plot to give the carbon content of each phase. Then go to the **'variables'** window, select **'F$LIQUID'** and copy it using the right-click menu.

Click on the lower plot, and in the **'Options'** window, edit the **'y-data'** line for the first series (**'series #0'**) of this plot. This should currently read **'X$LIQUID$C'**. Append **'*F$LIQUID'** to this.
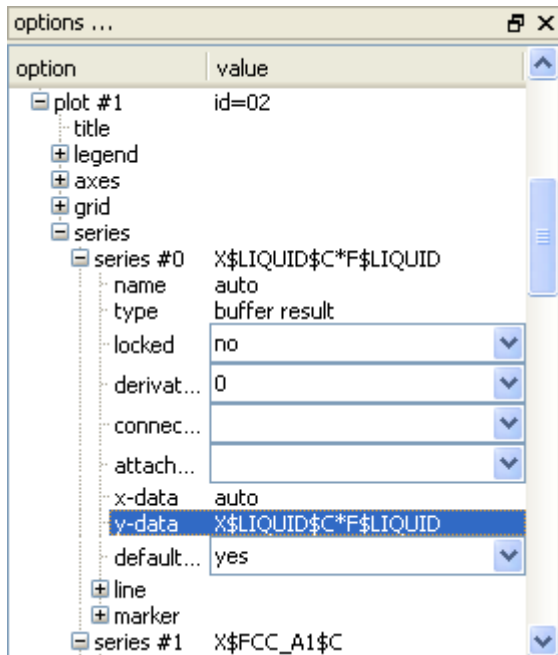
Repeat this process for the other series to give **'X\$BCC_A2\$C*F\$BCC_A2'**, **'X\$FCC_A1\$C*F\$FCC_A1'** and **'X\$CEMENTITE\$C*F\$CEMENTITE'**. Add another variable to the plot: **'XS\$C'** (can be found in the **'composition'** section), the mole fraction of carbon in the system. This should be equal to the sum of the other four variables on the plot.
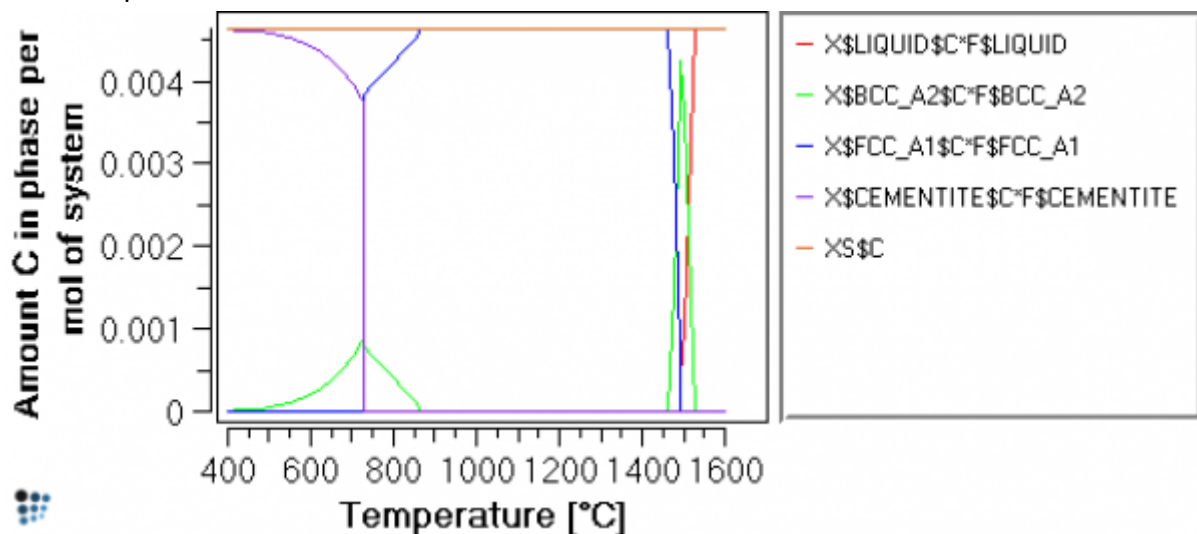
The final plot is shown below:

DEFINING FUNCTIONS

CREATING A NEW FUNCTION

If the expressions such as **'X\$BCC_A2\$C*F\$BCC_A2'** are likely to be used more than once, they can be defined as functions. Select **'Global > Variables & Functions'**. This brings up a box containing several tabs; click on **'Functions'**.

Click on **'New'** and type in a name for the function in the box which appears, for example, **'C_in_liquid'**. In the **'Expression'** box, type in **'X\$LIQUID\$C*F\$LIQUID'**. For convenience, this can be copied from the **'y-data'** line in the **'Options'** window of the plot just finished. (**N.B.**

There is no need to put an '=' sign at the beginning of the expression.) Click on **'Set'** to register the expression. Repeat for the three other expressions plotted above.
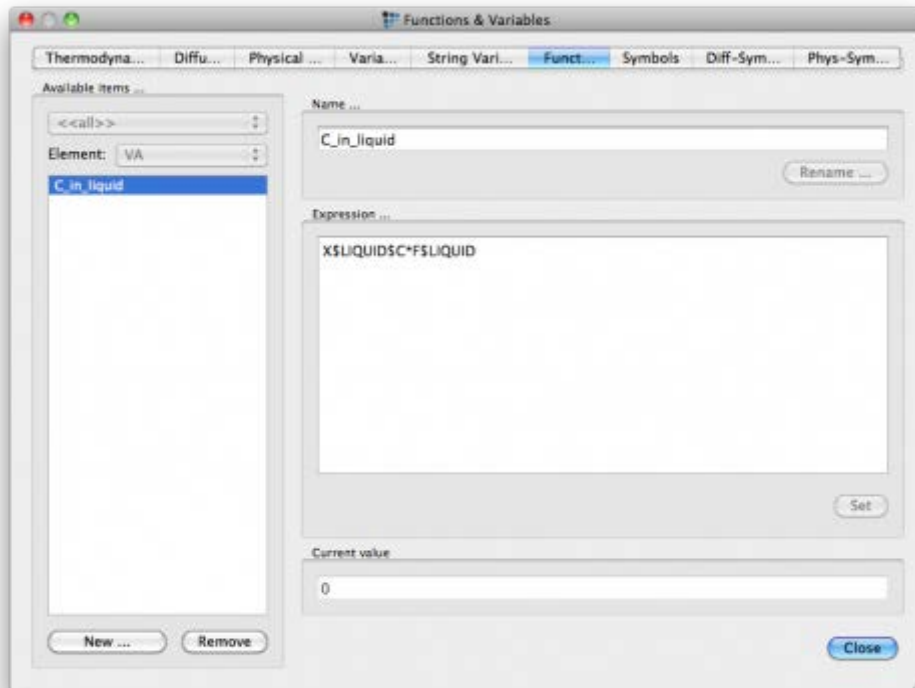
Close the **'Functions & Variables'** box to return to the main screen. Expand **'functions'** in the **'Variables'** window by clicking on the small plus-sign to the left of the word. This should give a list of the new functions:

Make a new plot and drag and drop the functions just defined into it, together with the **'XS$C'** variable, to check that this gives the same appearance as the plot above.

NEW EXPRESSIONS USING EXISTING FUNCTIONS

The fraction of the total carbon content in the system which is in the liquid phase can be calculated by dividing the function **'C_in_liquid'** by the total carbon content XS$C. Re-open the **'Functions and Variables'** tab and create a new function named **'Fraction_C_in_liquid'**. Enter **'C_in_liquid/XS$C'** in the **'Expression'** box and click on **'Set'**. Repeat for the other three phases.

On returning to the main screen, create a new plot and drag and drop the new **'Fraction_C_in…'** functions into it. (This may necessitate clicking on the **'minus'** sign by the side of **'Functions'** then clicking on the **'plus'** again to re-open it with the new functions

displayed.) The resulting plot should have the same appearance as the two plots above, but a different y-scale, this time going from 0 to 1.
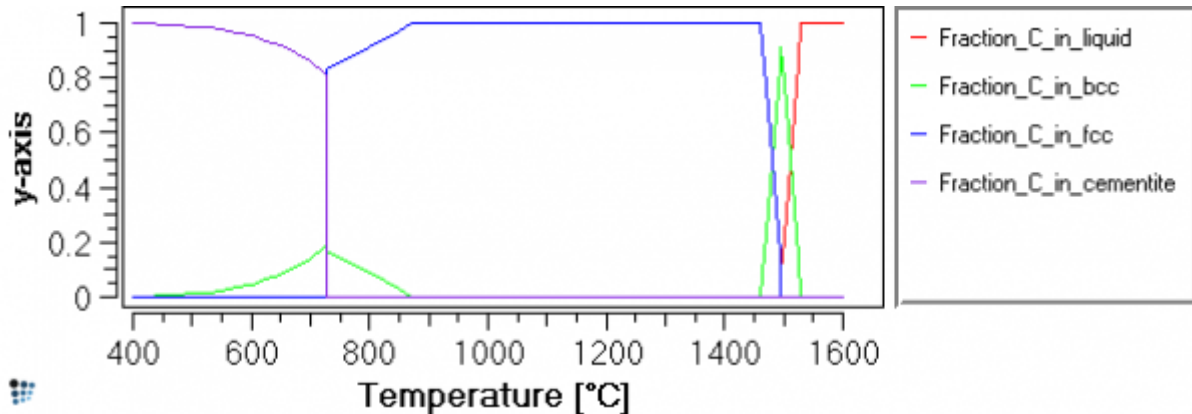
The user-defined functions are saved in the workspace and can be used for all subsequent calculations in that workspace.

Change the **'default x-data'** in the Options window to **'StepValue'**, and the name of the default x-axis to **'C content [wt.%]'**. Make a new stepped calculation in the **'_default_'** buffer, varying the carbon content from 0 to 0.5 wt.% (with 0.005 step) at 1475°C .

The phase fraction curve below shows that the carbon content has a strong influence on phase stability at this temperature. Increasing the carbon content stabilises FCC_A1 at the expense of BCC_A2, and then at higher carbon contents the liquid phase also becomes stable.
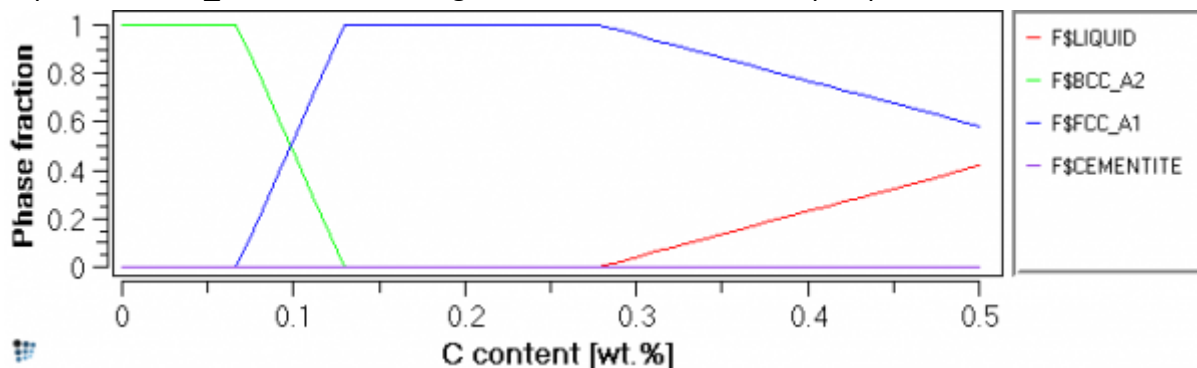
The two sets of user-defined functions appear as shown below, and in this case they provide different ways to illustrate the results.
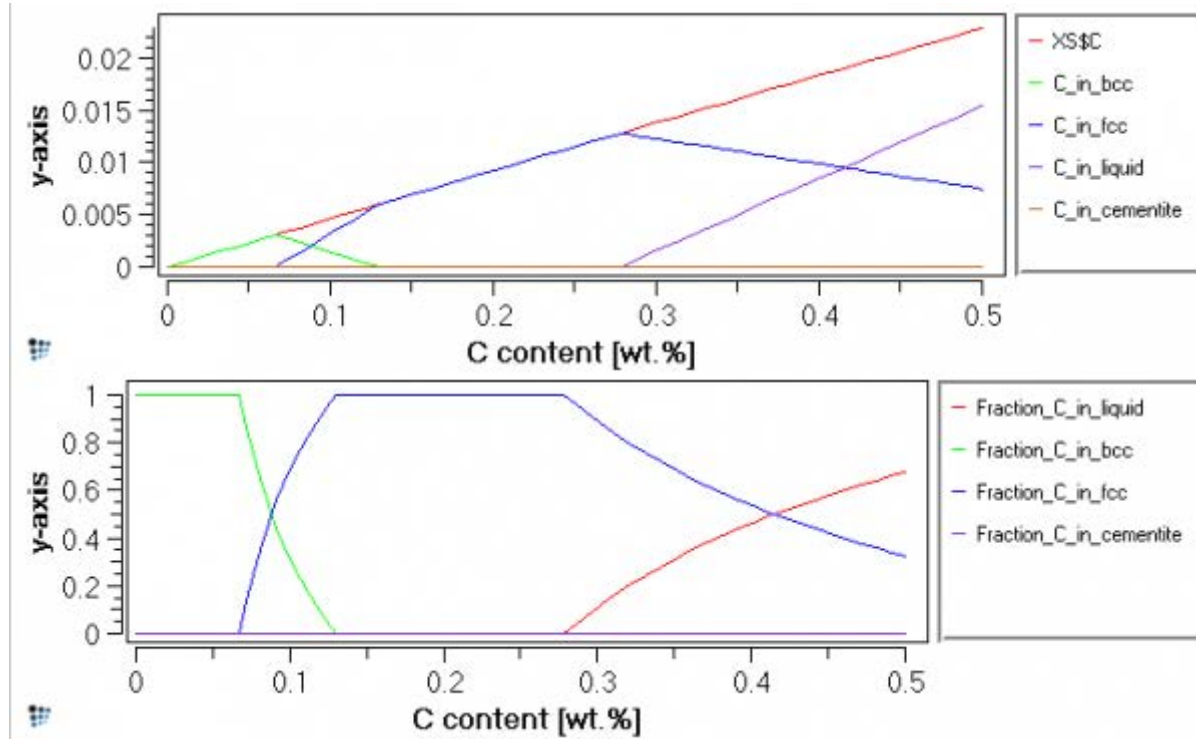
USER-DEFINED VARIABLES

The final part of this tutorial demonstrates the use of the **'Variables'** tab under **'Global > Variables & Functions'**.

In the plot of C_in_liquid, C_in_bcc, etc., the curves are made up of almost straight-line sections, so it should be possible to find analytical expressions of the form **y = ax +b** for these, where **'a'** is the gradient and **'b'** the intercept on the y-axis.

The C_in_liquid line starting from around 0.28 wt.% C will be used as an example. To find an equation for this line, two (x, y) values on the line are needed. For the first of these, y=0 can be used. To find the exact x-value at which the liquid phase fraction is zero, look at the **'Output'** window which contains now the equilibrium phases present in the system for various carbon contents. The line starting with **'Xsol 'LIQUID'** shows the LIQUID zero-phase boundary at 1475°C in terms of carbon content.

```
36, 0,00 s, 0,275, its 3, FCC_A1 - OK -
Xsol 'LIQUID': X(C): 0.012799895, WP(C): 0.2780809 - OK -
37, 0,02 s, 0,28, its 4, LIQUID FCC_A1 - OK -
```

The first (x, y) pair is therefore (0.2780809, 0). Go to **'Global > Variables & Functions'** and select the **'Variables'** tab. The variable **'x'** is already shown in the left-hand column. This is the StepValue, and currently has a value of 0.5.

Click on **'New'** and in the box, type in **'x1'**. Select it (in the **'Available items'** box) and type in or paste the first x-value (0.2780809) in the **'Expression'** box (confirmed by clicking on **'Set'**). Add another variable **'y1'**. This has a default value of zero, which does not need to be changed.
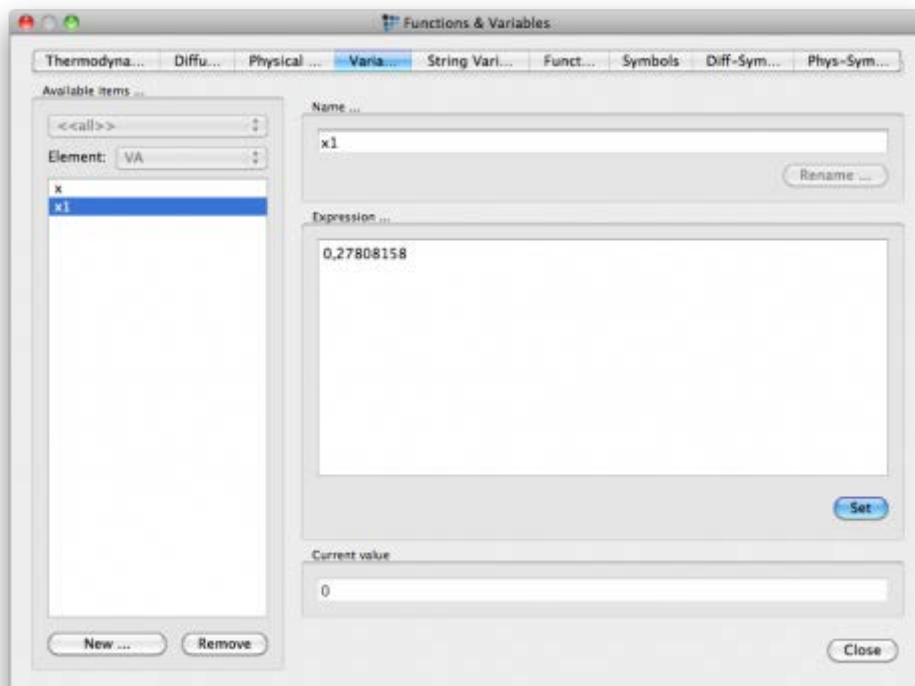
The second (x, y) pair can be obtained by finding the y-value at x=0.5. Either use edit the buffer state for this composition (**'Global > Buffers > Edit buffer state'**, click on **'0,5'** in the **'Buffer'** box) or simply set the composition to 0.5 wt.% C and calculate an equilibrium. In both cases, the value of **'C_in_liquid'** at this composition can be seen in the **'Variables'** window. Go to **'View > Create New Window'** and choose **'d1: List variable'**. Drag and drop **'C_in_liquid'** from the **'Variables'** window into the new **'List variables'** window which appears.

`C_in_liquid +1.536688764453e-002`

The numerical value can be selected and copied from this window. Re-open the 'Variables' tab and add the new variables **'x2'** and **'y2'**, equal to 0.5 and 1.536688764453e-002 respectively.

The slope **a** and intercept **b** of the straight line can now be entered; **a** is equal to **(y2-y1)/(x2-x1)** and **b** to **((x2*y1)-(x1*y2))/(x2-x1)**. Create a new variable named **'a'**, type in the formula (or try to copy it from this tutorial) and click on **'Set'**. This evaluates the expression and places the numerical value in the **'Expressions'** box in the place of the formula. Do the same for **'b'**. In the **'Functions'** tab, the equation of the line can now be entered. Create a new function **'Liquid_line'** and type **'(a*x)+b'** into the **'expression'** box. Click **'Close'** to return to the main screen.

Drag the new **'Liquid_line'** function from the **'Variables'** window to the plot of **'C_in_liquid'**, etc.

The resulting plot should look like this:
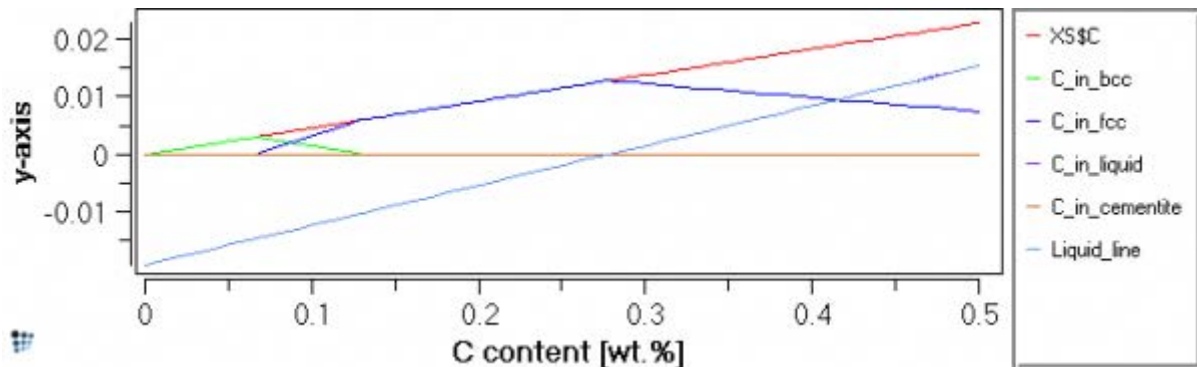
The **'Liquid_line'** function extends to negative values, unlike the true C_in_liquid curve, which has a value of zero for carbon contents between zero and 0.27 wt.%.

One way of removing the unwanted part of this line is to select **'Edit series data'** from the right-click menu. In the resulting table of **'Liquid_line'** series, select all the rows for which the y-value is negative and then click on **'Delete rows/cols'** to remove them. Accept the warning with **'OK'**.

An alternative way is to add the series as a **'function/expression'** rather than as a **'buffer result'**. There are differences in the way the program treats these two types of series; for example, in a **'function/expression'** series, x-values are specified as a numerical range, and the y-values are functions of x, whereas for **'buffer results'**, the x-values are specified as a variable (by default, the StepValue), and the y-values as another variable.

When a variable is dragged and dropped from the **'variables'** window, it automatically becomes a **'buffer result'**-type series. To add a **'function/expression'** series, click on the plot, then in the options window, select **'new series'** from the right-click menu, and choose **'function/expression'**. By **'y-data'** for the new series, type in **'Liquid_line'**. Edit the **'x-data'** line to type **'x1..0.5'**.
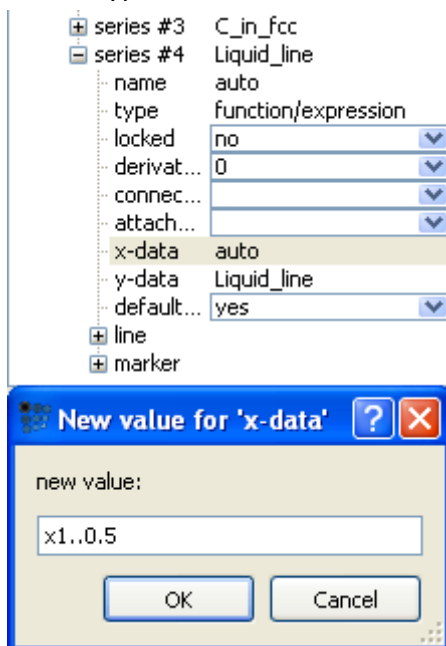
The plot should now look as shown in the image below (with the **'Liquid_line'** series highlighted).
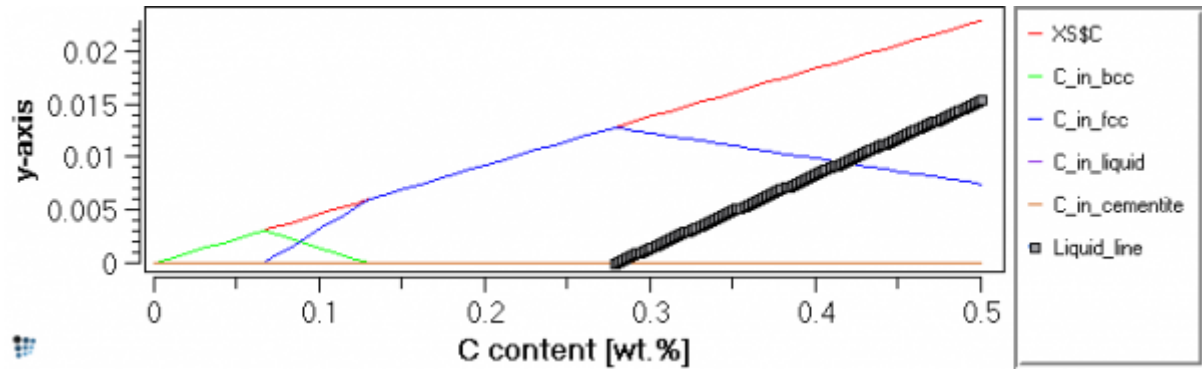
CONSECUTIVE ARTICLES

The tutorial is continued in article T7 - Calculating transformation temperatures and phase boundaries

T7: Calculating phase boundaries

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb

Contents

- Using "Search phase boundary" with temperature variation to determine solidus and liquidus
- Determining austenite ⟷ ferrite transformation temperatures
- Finding phase boundaries for carbide phases in terms of temperature and element content
- Tracing a phase boundary on axes of temperature versus element content

It was seen in Tutorial 3 that MatCalc evaluates solubility temperatures (Tsol) or compositions (Xsol) during the course of stepped equilibrium calculations. It is also possible to calculate these individually using the **'Search phase boundary'** function.

Setting up the system

Create a new workspace file and set up the system with elements **Fe**, **C** and **Nb** and phases **FCC_A1**, **BCC_A2**, **LIQUID** and **CEMENTITE**. Enter the composition as 0.1 wt.%C, 0.3 wt.% Nb and calculate an equilibrium at 1000°C (Refer to Tutorial 1 and Tutorial 2 if necessary.)

Note the results in the **'Phase details'** window. A second FCC_A1 phase has automatically been created, and examination of its composition shows that its approximate formula is NbC.

```
#### /FCC_A1/ moles: 0.99669, gm: -62332.5 (-62332.5), sff: 0.996959
Phasestatus: entered - active
FE +9.96862e-001 C +3.04146e-003 NB +9.65336e-005
#### /FCC_A1#01/ moles: 0.00331011, gm: -112964 (-112964), sff: 0.514554
Phasestatus: entered - active
NB +5.14395e-001 C +4.85446e-001 FE +1.59075e-004
### inactive ###
#### /BCC_A2/ moles: 0, gm: -62262.4 (-62262.4), sff: 0.999701
Phasestatus: entered - not active (dfm=-82.83)
FE +9.99572e-001 C +2.99142e-004 NB +1.28377e-004
#### /LIQUID/ moles: 0, gm: -58601.3 (-58601.3), sff: 1
Phasestatus: entered - not active (dfm=-3777)
FE +9.75342e-001 C +2.34127e-002 NB +1.24518e-003
#### /CEMENTITE/ moles: 0, gm: -52390.6 (41804.9), sff: 0.25
Phasestatus: entered - not active (dfm=-9077)
FE +7.50000e-001 C +2.50000e-001 NB +6.86915e-008
```

It is the following line in the database file **mc_sample_fe.tdb** which causes the second FCC_A1 phase to be created:

```
ADD_COMPOSITION_SET FCC_A1 :TI,NB,V:C,N: !
```

This creates that a **new phase of type FCC_A1** with Ti, Nb or V as the major constituents on the first sublattice and C or N as the major constituents on the second when the system contains these elements. The **'General'** tab in the **'Phase status'** box (**'Global > Phase status'**)

shows the major constituents for each phase, :FE:VA: and :NB:C: respectively for FCC_A1 and FCC_A1#01.

CALCULATING PHASE BOUNDARIES

SOLIDUS AND LIQUIDUS TEMPERATURES

The solidus temperature is defined by zero phase fraction of liquid. To calculate this, choose **'Search phase boundary'** from the **'Calc'** menu or click on the ⬚ icon. The box below appears. Select **'Temperature'** in the left-hand column and **'LIQUID'** in the **'Target phase'** column, then click on **'Go'**.
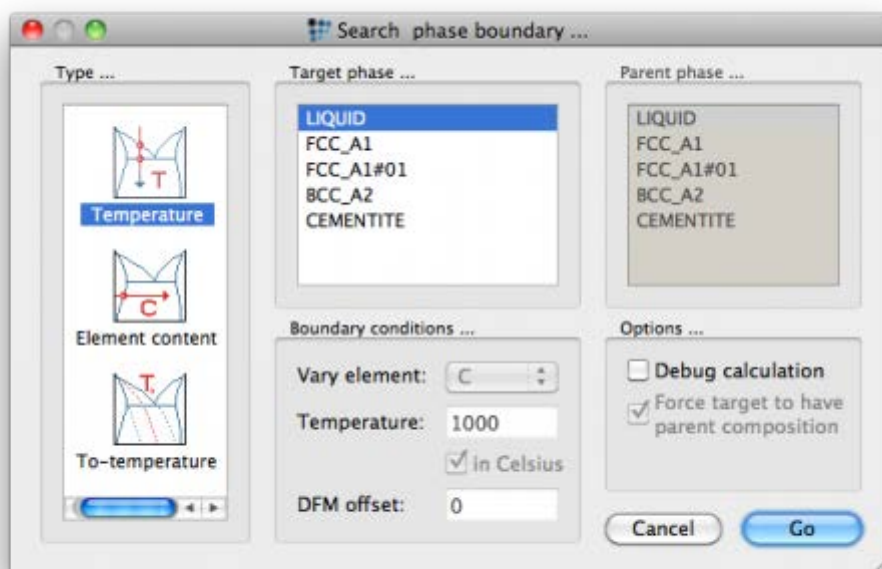
The following message appears in the output window.

`Tsol 'LIQUID': 1480.30 C (1753.46 K) iter: 16, time used: 0.02 s`

The liquidus temperature is the dissolution temperature of the last solid phase, which in this case is BCC_A2. Selecting **'BCC_A2'** as the target phase gives the following result:

`Tsol 'BCC_A2': 1452.43 C (1725.59 K) iter: 5, time used: 0.00 s`

Of course, this is not a liquidus temperature, as it cannot be lower than the solidus temperature. This result is given because MatCalc finds the zero phase fraction temperature of BCC_A2 phase next to the temperature of the last calculation which is 1480.30°C in this case (the liquidus temperature). Information given in **'Phase summary'** window explains that at 1452.43°C, BCC_A2 appears next to FCC_A1 phase (inactive BCC_A2 phase has the driving force value of zero). **It is recommended to look at the 'Phase summary' window in order to check if the found phase boundary is the desired one!**

The liquidus phase can be easily found if an equilibrium calculation in the liquid system is performed first. Calculate an equlibrium at 1600°C (or any temperature in which system contains only a liquid) and search again for the phase boundary of BCC_A2 phase. This time the following result should be given:

```
Tsol 'BCC_A2': 1527,33 C (1800,49 K) iter: 4, time used: 0,03 s
```
In general, the correct phase boundaries are found if the initial equilibrium describes the system in the neighbouring phase field which does not contain the searched phase - in the case presented above, the liquidus temperature (which is the border between the "BCC+LIQUID" and "LIQUID" phases) was found from the "LIQUID" phase field. Also, the algorithm used to search for phase boundaries might fail to converge if the starting point is too far away from the boundary.

AUSTENITE-FERRITE TRANSFORMATION TEMPERATURES

Low-alloy steels undergo a ferrite - austenite phase transformation between 700 and 800°C (see, for example, Tutorial 4). To find the exact temperatures of the transformation in the Fe-0.1wt.%C-0.3wt.%Nb system, calculate an equilibrium at 700°C and use again **'Search phase boundary'**. Select **'FCC_A1'** as a target phase to identify the zero-phase boundary temperature for austenite.
```
Tsol 'FCC_A1': 726.62 C (999.78 K) iter: 11, time used: 0.00 s
```
The zero-phase boundary of BCC_A2 for this transformation can be identified by calculating an equilibrium at 900°C and then searching for the boundary.
```
Tsol 'BCC_A2': 883,07 C (1156,23 K) iter: 5, time used: 0,05 s
```

DISSOLUTION TEMPERATURES OF CARBIDES

Cementite is only stable to relatively low temperatures, so calculate an equilibrium at 800°C as a starting point, then search for the phase boundary.
```
Tsol 'CEMENTITE': 726,62 C (999,78 K) iter: 9, time used: 0,05 s
```
Note that this is the same temperature as the zero-phase boundary of FCC_A1. Niobium carbide, by contrast, remains stable at higher temperatures. Calculate an equilibrium at 1400°C before searching for the boundary.
```
Tsol 'FCC_A1#01': 1346.00 C (1619.16 K) iter: 5, time used: 0.00 s
```

ELEMENT CONTENT FOR ZERO-PHASE FRACTIONS

Phase boundaries can also be found in terms of element content at a fixed temperature. To illustrate this, the zero-phase boundary of cementite at 700°C will be evaluated in terms of carbon content. Calculate an equilibrium at 700°C, then open the **'Search phase boundary'** box and select **'Element content'** in the left-hand column. Set the target phase to **'CEMENTITE'**, the element to be varied to **'C'**, and the temperature to **'700'**, then click **'Go'**.
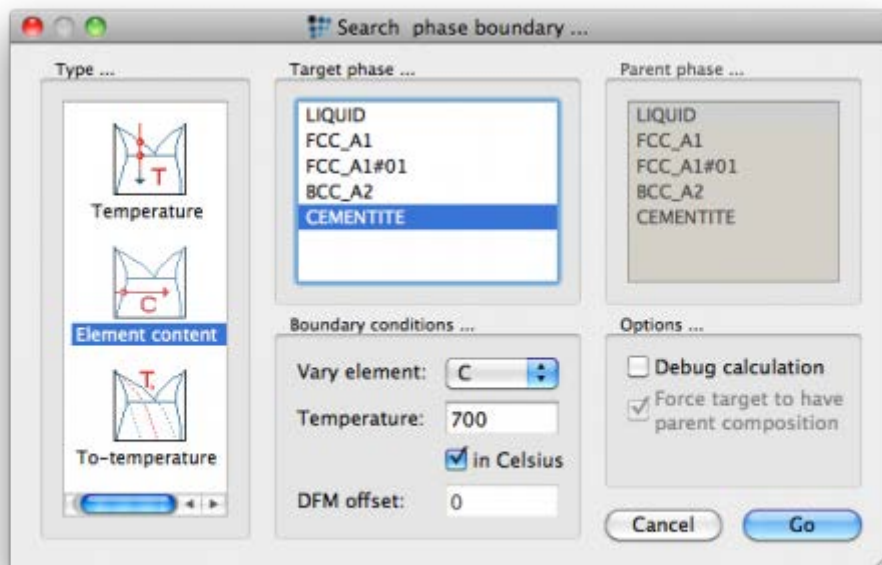
The output gives the carbon content for zero phase fraction of cementite in mole fraction and in weight percent.

```
iter: 2, time used: 0.00 s, GibbsEnergy: -40682.343 J
X(C): 0.0024577437, WP(C): 0.052897424, T: 700 C (973.16 K) - OK -
```

Note: After the search for the phase boundary with element content variation, the composition of the system is changed to the found value! (check 'Global > Composition')

In the same way, the zero phase fraction boundary for niobium carbide at 1000°C can be evaluated in terms of the niobium content. Firstly, open **'Global > Composition'** and reset the carbon content to **0.1 wt.%**. Calculate an equilibrium at **1000°C**, then search for the phase boundary for **'FCC_A1#01'**, this time setting the element to be varied to **'Nb'**.

```
iter: 7, time used: 0.02 s, GibbsEnergy: -62319.956 J
X(NB): 6.653432e-005, WP(NB): 0.011108476, T: 1000 C (1273.16 K) - OK -
```

TRACING PHASE BOUNDARIES

Once a point on a phase boundary has been identified using the process described above, the boundary can be traced as a function of element content. In the following example, the effect of the niobium content on the temperature of the FCC_A1#01 (NbC) zero-phase boundary will be calculated.

Having established the zero phase fraction boundary for niobium carbde at 1000°C, open the **'Step equilibrium'** window using **'Calc > Stepped calculation'** and select **'Phase boundary'** from the left-hand column.

In the **'Boundary conditions'** box, set the element to **'Nb'**, the target phase to **'FCC_A1#01'** and the max. T-step to **'100'**. (The use of this parameter will be discussed in Tutorial 8.) Enter **'0.01'**, **'0.6'** and **'0.01'** as the start, stop and step interval values in the **'Range'** box. Click on **'Go'** to perform the calculation
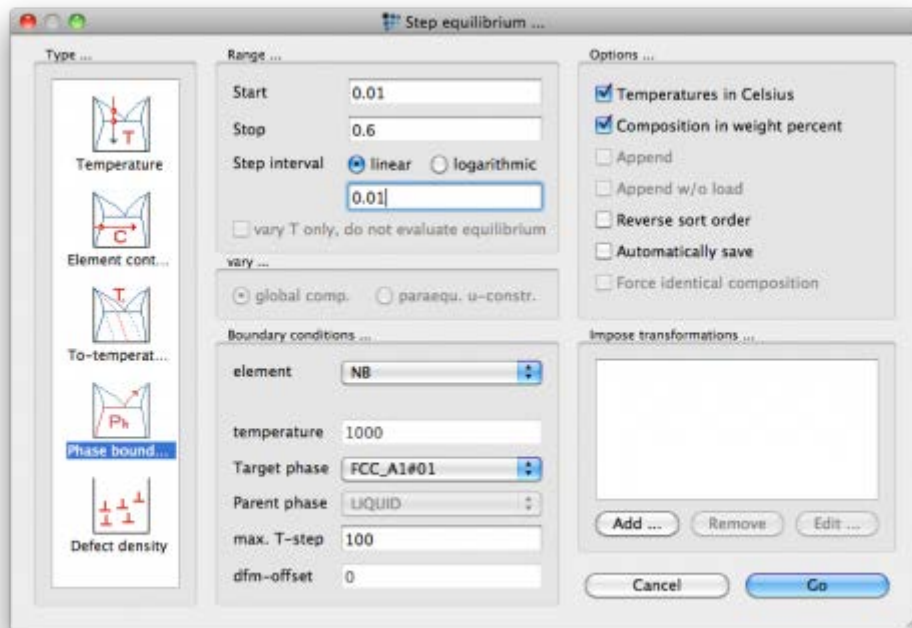
Create a new X-Y plot window (Tutorial 4) and drag and drop **'T$c'** (from **'favorites'** category in variables window) into it. The plot should look like this:
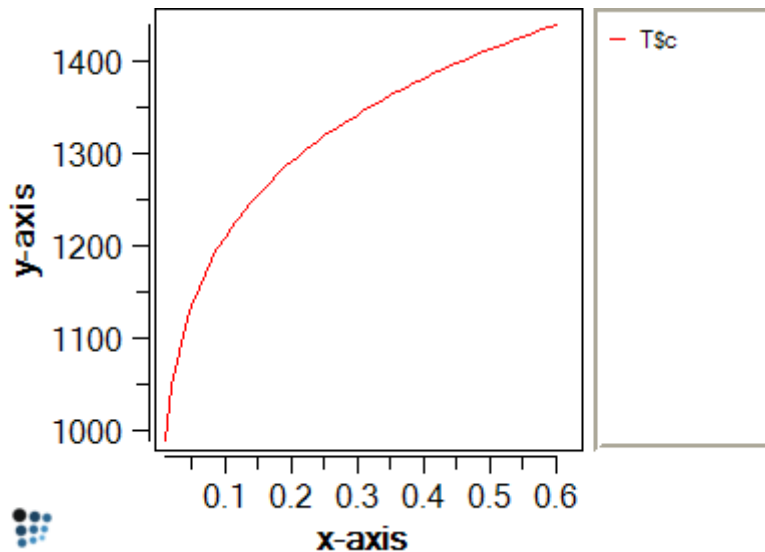
Right-click in the plot window outside the plot area and choose **'Duplicate and lock series'** from the window (see Tutorial 5). Double-click on the name of the series to duplicate it. In the **'Options'** window, change the name of the original series (**'*_T$c'**) to **'0.1 wt.%C'**. Change the carbon content of the system to 0.05 wt.% C, calculate an equilibrium at 1000°C and search again for the same phase boundary, then make a stepped calculation using the same conditions as before. The phase boundary for 0.05 wt.% C should follow the green curve in the plot below, which also shows the same phase boundary for 0.01 wt.%C.
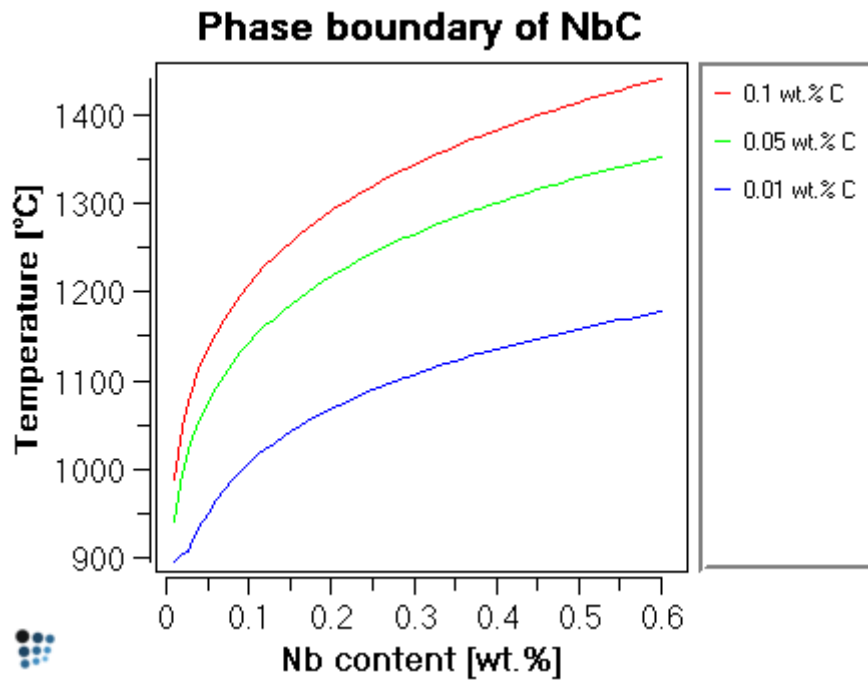
CONSECUTIVE ARTICLES

The tutorial is continued in article T8 - Calculating a phase diagram in a binary system

T8: Calculating a phase diagram in a binary system

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb

This tutorial introduces the calculation of phase diagrams with an example featuring the well-known Fe-C binary system.

Contents:

- Calculating phase boundaries
- Building up the phase diagram from the calculated boundaries
- Choosing appropriate calculation parameters
- Phase diagrams using stable and metastable equilibria

A phase diagram consists of a number of phase-boundaries separating regions of temperature- and composition-space in which different phases are stable at equilibrium. Published equilibrium diagrams for the Fe-C system often show equilibria between Fe-rich phases and both C (in the form of graphite) and cementite (Fe_3C). Graphite is the more stable of these two phases, and forms readily in cast irons (2-4 wt.% C), but usually with great difficulty in steels (up to 1.5 wt.% C). In the latter, it is more practically useful to consider metastable equilibria involving Fe_3C. In this tutorial, phase diagrams for both Fe-C and Fe-Fe_3C will be calculated.

Setting up the system

Create a new workspace file. From the **'mc_sample_fe.tdb'** database, select the elements FE and C and the phases LIQUID, BCC_A2, FCC_A1, CEMENTITE and GRAPHITE. Enter the composition 0.05 wt.% C. Create a new plot window of type p1 (X-Y data). The phase diagrams will be calculated from 0 to 5 wt.% C, but the low carbon content of 0.05 wt.% C is chosen so that the lines bounding the high-temperature ('delta') ferrite phase, which is only stable at relatively low carbon contents, can be found. Firstly, the Fe-Fe_3C diagram will be calculated, so it is necessary to suspend graphite, since it is more stable than Fe_3C. Open **'Global > Phase status'**. In the **'General'** tab, put a tick-mark in the box beside **'suspended'**:

Fᴇ-Fᴇ₃C ᴘʜᴀsᴇ ᴅɪᴀɢʀᴀᴍ
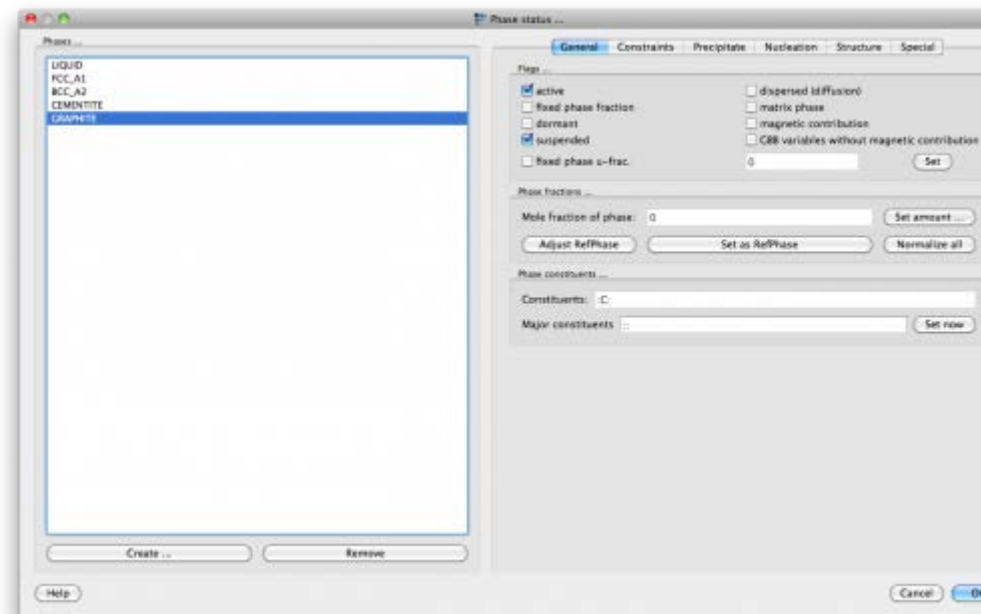
The phase diagram is made up of a number of phase boundaries. As was have seen in the last part of Tutorial 7, these boundaries can be found by finding a point on the boundary, then tracing the boundary as a function of element content. The method for tracing a boundary for phase **'X'** is as follows:

1. Calculate an equilibrium at an appropriate temperature, near to the expected boundary temperature
2. Find the 'X'-phase boundary by varying the temperature with 'X' as the target phase
3. Perform a stepped calculation, varying the element content between selected limits, with 'X' as the target phase

Uᴘᴘᴇʀ ʙᴏᴜɴᴅᴀʀʏ ᴏғ ᴅᴇʟᴛᴀ-ғᴇʀʀɪᴛᴇ, BCC_A2

Beginning at the high-temperature end of the diagram, the uppermost phase boundary at a composition of 0.05 wt.% C is between a single-phase liquid region and a liquid and delta-ferrite (BCC_A2) region. The first boundary which must be found is, therefore, a BCC_A2 phase boundary.

To locate the boundary, an equilibrium must first be calculated reasonably close to the expected boundary temperature. It can be seen that the line lies somewhere between 1538°C (the melting temperature of pure iron) and 1500°C. Click on the 🔆 icon and enter the temperature **'1530'**. (If this gives an error message, select **'Calc > Set start values'** then repeat the equilibrium calculation.) Then click on 📈 to open the **'Search phase boundary'** window. Select **'Temperature'** in the left-hand column and **'BCC_A2'** as the target phase. The 'Output' window should show the following message:

```
Tsol 'BCC_A2': 1533.98 C (1807.14 K) iter: 4, time used: 0.00 s
```

This shows that a point on the boundary has been found successfully. The next step is to trace this boundary using the stepped equilibrium function to vary the carbon content. Click on 💡... and choose **'Phase boundary'** from the left-hand column. Enter the range: **'0'** to **'5'**, in intervals of **'0.01'**. Select **'C'** as the varying element and **'BCC_A2'** as the target phase. Leave the **'Max T-step'** value at its default value of **'20'**. In the **'Options'** section of this window, check that **'Temperature in Celsius'** and **'Composition in weight percent'** are both selected. Click on **'Go'** to launch the calculation.
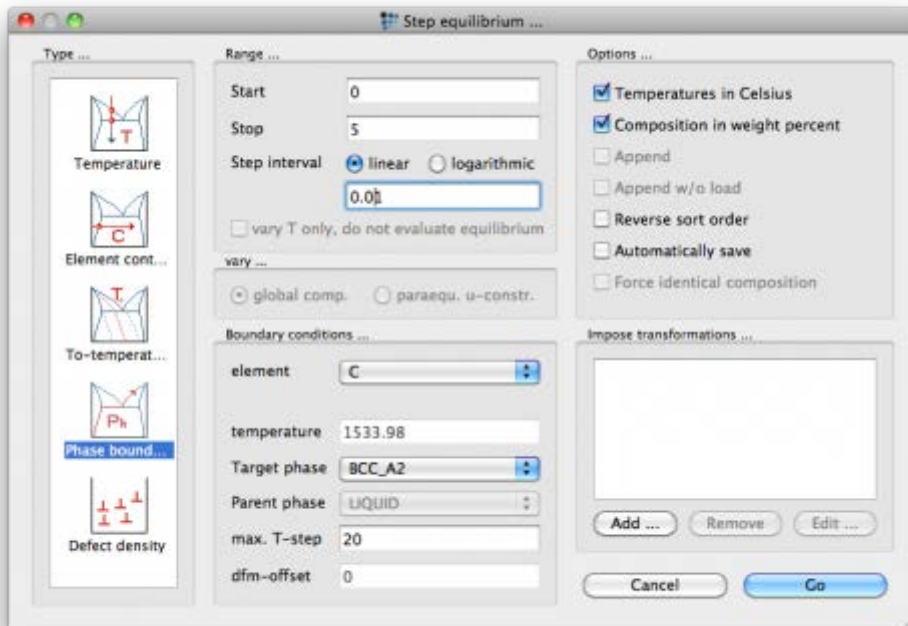
The following message appears ; accept it with **'Yes'**.

Now that the first phase boundary has been calculated, drag and drop **'T$C'** from the **'Variables'** window (where it can be found under **'favorites'**) to the plot. It is useful to add gridlines to the plot. Note that the x-axis currently only runs from zero to just over 0.5 wt.% C. From the point identified on the phase boundary, the calculation first proceeds in a direction of increasing carbon content. However, the BCC_A2 phase is not stable beyond approx 0.53 wt.% C, so the calculation (which cannot reach the stop limit of 5 wt.% C) stops and the

'Continue in other direction?' message shown above is displayed to ask whether the user wishes to complete the rest of the calculation, in which the carbon content is decreased from the point identified at 0.05 wt.% C to zero.
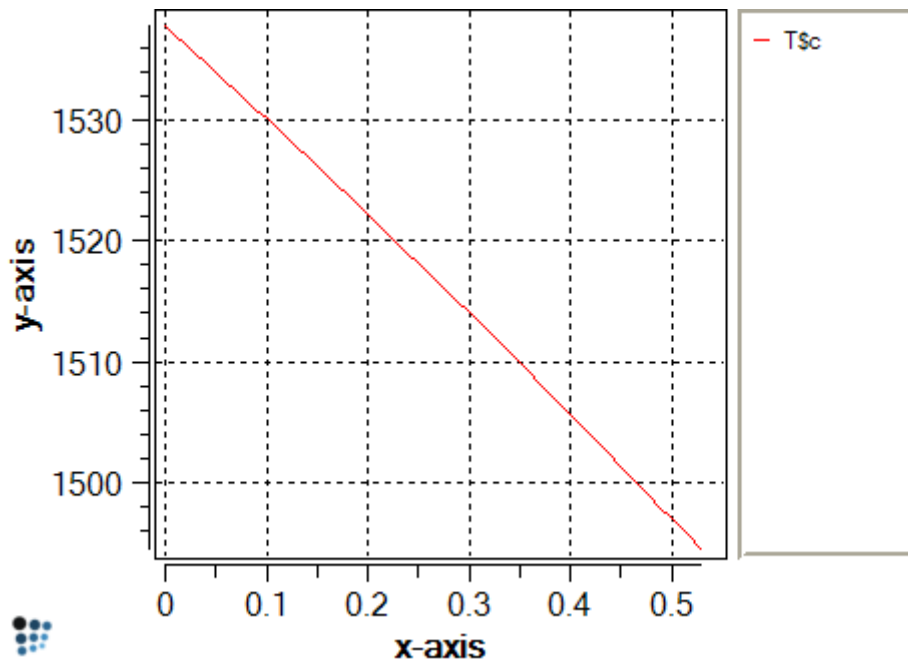
Right-click in the plot window outside the plot area itself, and select **'Duplicate and lock series'** from the menu displayed. Select the name of the series and click **'Duplicate'** to produce a copy of the series. In the **'options'** window, rename the first series **'bcc_high_1'**.

LOWER BOUNDARY OF LIQUID

The next phase boundary encountered on decreasing the temperature is between the LIQUID + BCC_A2 region and the BCC_A2 single-phase region, so this is a LIQUID-phase boundary. 1500°C would appear to be a suitable temperature for the starting equilibrium to find this line. In the **'search phase boundary'** box, select **'LIQUID'**. The following line of output should appear:

`Tsol 'LIQUID': 1515.43 C (1788.59 K) iter: 4, time used: 0.00 s`

Then make a stepped calculation with the same start, stop and interval values and the target phase set to **'LIQUID'**. (A start-value of zero is automatically changed by the program to **'1e-9'** to facilitate the calculation.)

The diagram should now look like this:
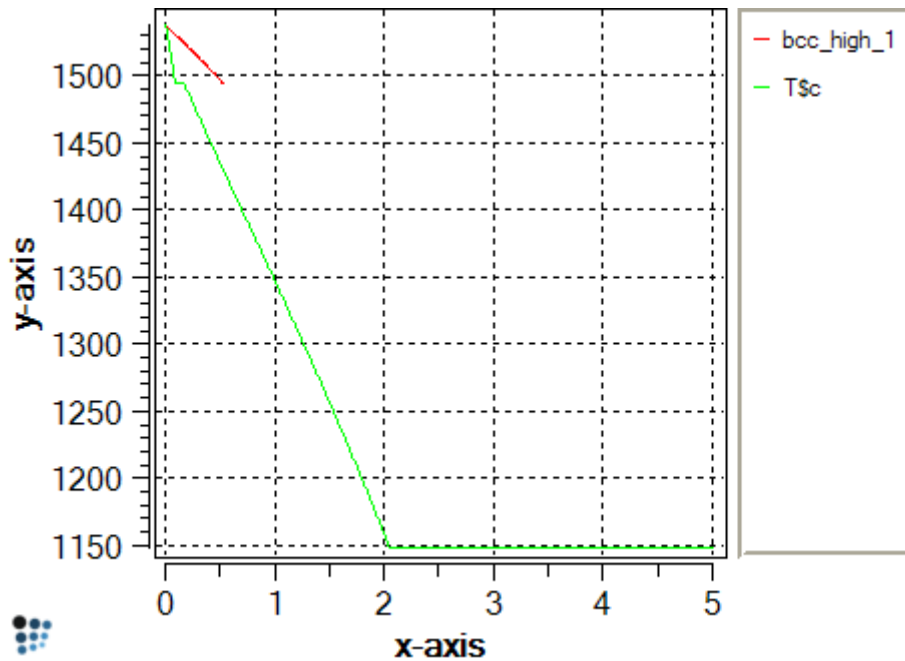
LOWER BOUNDARY OF DELTA-FERRITE (BCC_A2)

Calculate an equilibrium at 1400°C, search for BCC_A2 (the boundary temperature should be 1429.60 C (1702.76 K)), step from 0 to 5 wt.% C with an interval of 0.01 wt.% C. Accept the **'Continue in other direction'** message (the calculation could not reach 5 wt.% C limit, again) with **'Yes'**.

UPPER BOUNDARY OF AUSTENITE (GAMMA, FCC_A1)

Calculate an equilibrium at 1500°C, search for FCC_A1, step from 0 to 5 wt.% C with an interval of 0.01 wt.% C. The boundary temperature should be 1460.18 C (1733.34 K).

UPPER BOUNDARY OF LOW-TEMPERATURE ('ALPHA') FERRITE, BCC_A2
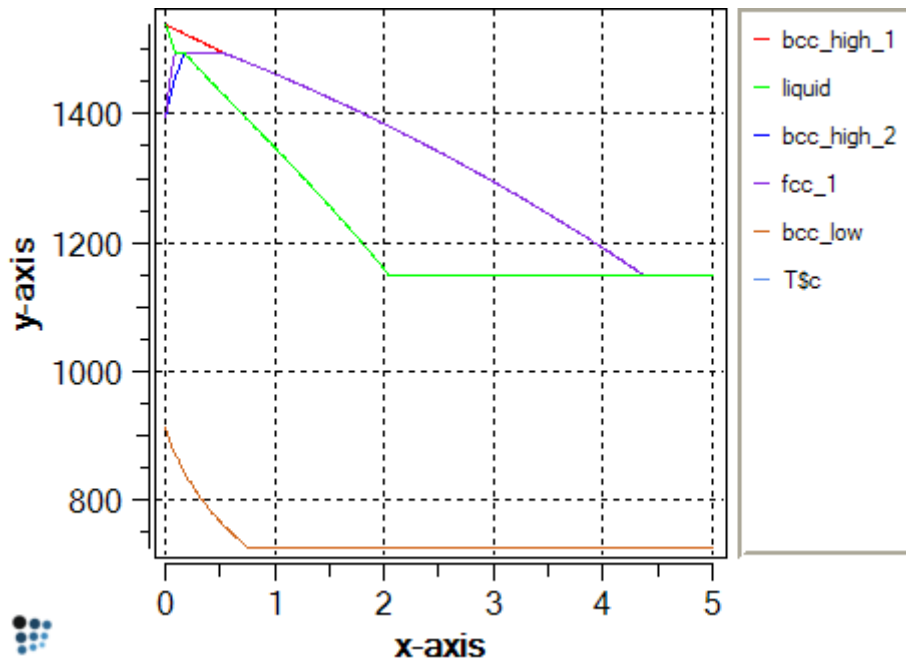
Calculate an equilibrium at 900°C, search for BCC_A2, step from 0 to 5 wt.% C with an interval of 0.01 wt.% C. The boundary temperature should be 888.64 C (1161.80 K).

The image below shows how the diagram should look, with appropriate labels for the lines:

The most of the upper section is now done, with the exception of the phase boundary between LIQUID and LIQUID + CEMENTITE for hypereutectic compositions. This line is continuous with the cementite line between the FCC_A1 and FCC_A1 + CEMENTITE regions and the horizontal line between BCC_A2 + FCC_A1 and BCC_A2 + CEMENTITE regions, so it will appear when this line is calculated.

In the lower section, there is a very narrow alpha-ferrite single-phase region at low carbon contents. The upper part of this region is bounded by an FCC_A1 boundary, and the lower part of the region by a CEMENTITE boundary. Since these two boundaries are very steep, it is necessary to modify the calculation parameters. Failure to do this can lead to incorrectly calculated boundaries, as shown in the diagram below (an attempt to calculate the FCC_A1 line using the parameters used so far).
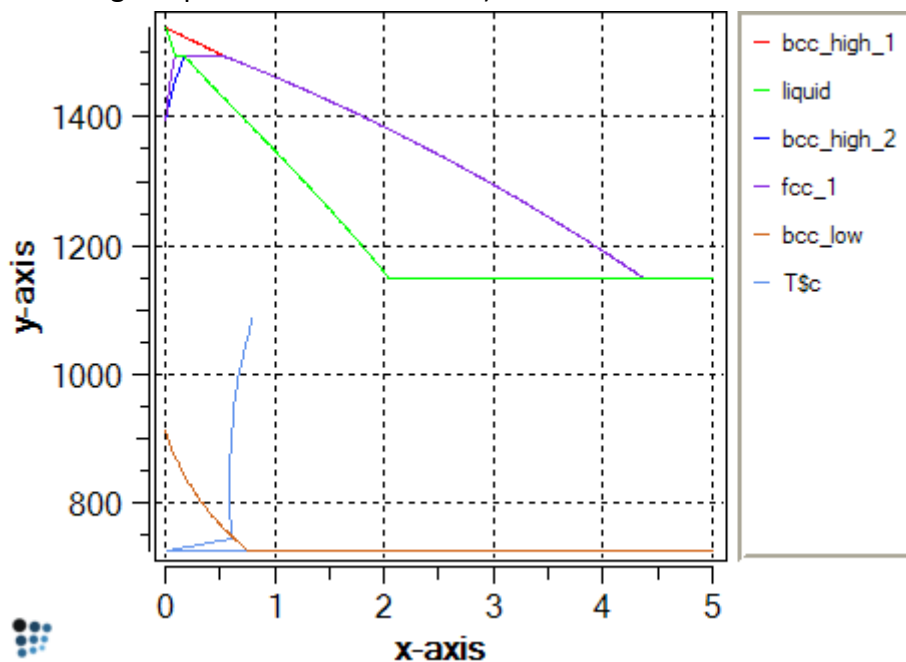
Lower boundary of austenite (gamma, FCC_A1)

Calculate an equilibrium at 600°C then search for the FCC_A1 phase boundary, which should be at 726.62°C. Step from 0 to 5, with an increment of 0.001 instead of 0.01. This reduced increment makes the calculation rather more time-consuming; on a slow machine, it may be better to divide it into two parts: step from 0 to 0.02 with an increment of 0.001, duplicate and lock, step from 0.02 to 5 with an increment of 0.01.

Upper boundary of cementite

Calculate an equilibrium at 800°C. Search for the CEMENTITE phase boundary; this also should be at 726.62°C. Using the same settings as for the previous stepped calculation, the phase boundary is calculated correctly, but extends in the negative temperature direction beyond physically reasonable values. This occurs because the calculated boundary becomes increasingly steep as the carbon content approaches zero.

One way of removing the unwanted line portion is simply to modify the scaling of the y-axis. (The minimum temperatures given on equilibrium diagrams are typically 400-500°C, because it becomes difficult to attain equilibrium over practical timescales at low temperatures.) Another solution is to remove unwanted data points using 'Edit series data' from the right-click menu of the plot.

Alternatively, the **'overshoot'** can be avoided by modifying the parameters of the stepped calculation. Increasing the **'max T-step'** allows greater steps in temperature, enabling the program to cope with very steep boundaries. A suitable value is 100 or 200. Additionally, setting the starting value of the stepped calculation to a slightly higher value, for example 0.0005 instead of 1e-9, avoids the calculation of the steepest parts of the phase boundary. With these modified settings, a satisfactory appearance is obtained without the need to change the axis scalings or delete any points.

## A few words on the 'max. T-step' parameter

Following a phase boundary in the stepped calculation is performed by a simple procedure. Once an initial point is found with **'Search phase boundary'** operation, the composition of the system is changed by a value specified as a step in the **'Range'** section of **'Stepped equilibrium'** window. For this new composition, MatCalc search a phase boundary in a temperature range **(T_{old} - 'max T-step' ; T_{old} + 'max T-step')**, where **T_{old}** is a temperature of a phase boundary at a previous composition. If the phase boundary is too steep, no phase boundary would be found. In such a case MatCalc changes a variable from the element content to the temperature (this is indicated by the message **'changing independent variable to temperature'** in the **'Output'** window). In effect, the temperature will be varied by a step equal to the value of **'max T-step'** parameter and MatCalc will look for the phase boundary at that temperature. In some cases, this might result with the wrong equilibria, especially when the stoichiometric compounds are the equlibrium phases (due to the undefined chemical potentials for these phases).

THE FINISHED DIAGRAM

Do not forget to lock the last series to be added, so that it is not modified when another calculation is performed. Add axis labels and a title **'Fe-Fe₃C phase diagram'**. The subscript can be obtained using HTML tags:

`Fe-Fe<sub>3</sub>C phase diagram`

The finished phase diagram should look like this; compare with the sketch below to verify that all the lines have been calculated correctly.
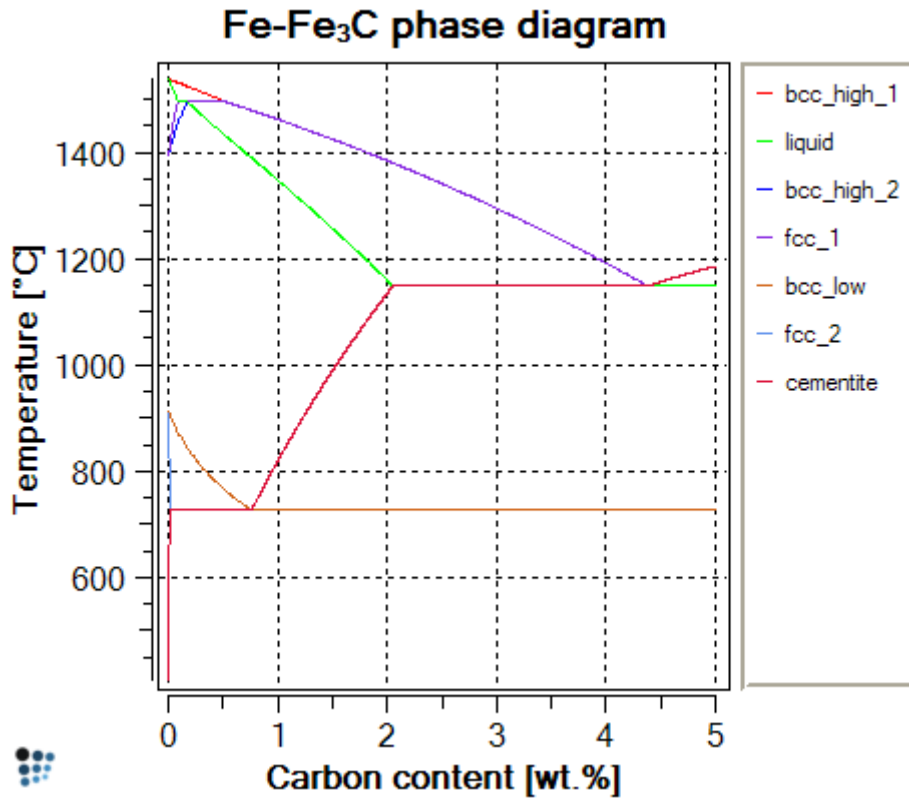
The image below shows an expanded version of the low-C region.

Fe-Fe₃C phase diagram
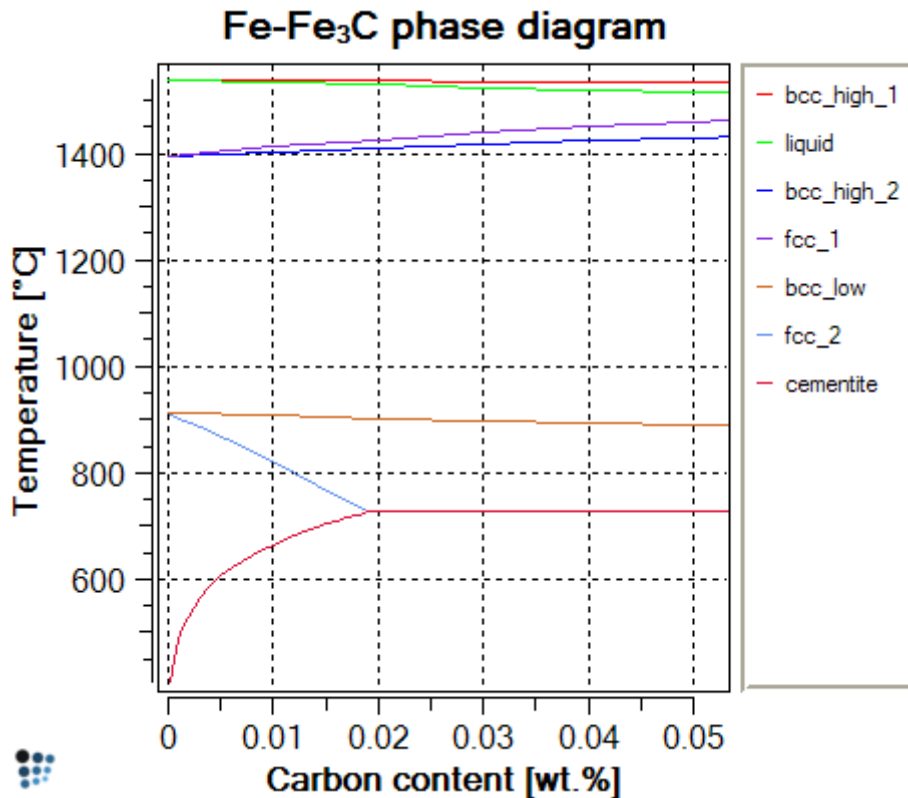
FE-C PHASE DIAGRAM

Set up this system by removing the **'suspended'** flag for GRAPHITE under **'Global > Phase status > General'**.

The calculation of the Fe-C diagram is left as an exercise to allow the user to familiarise him- or herself with the method, including the choice of appropriate values for the starting equilibrium calculation temperatures and the calculation parameters. However, suggestions are given at the foot of the page. The diagram below shows how the finished diagram should look. (Alternatively, the phase boundaries from the Fe-C calculations can be superposed on the Fe-Fe₃C phase diagram for comparison.)
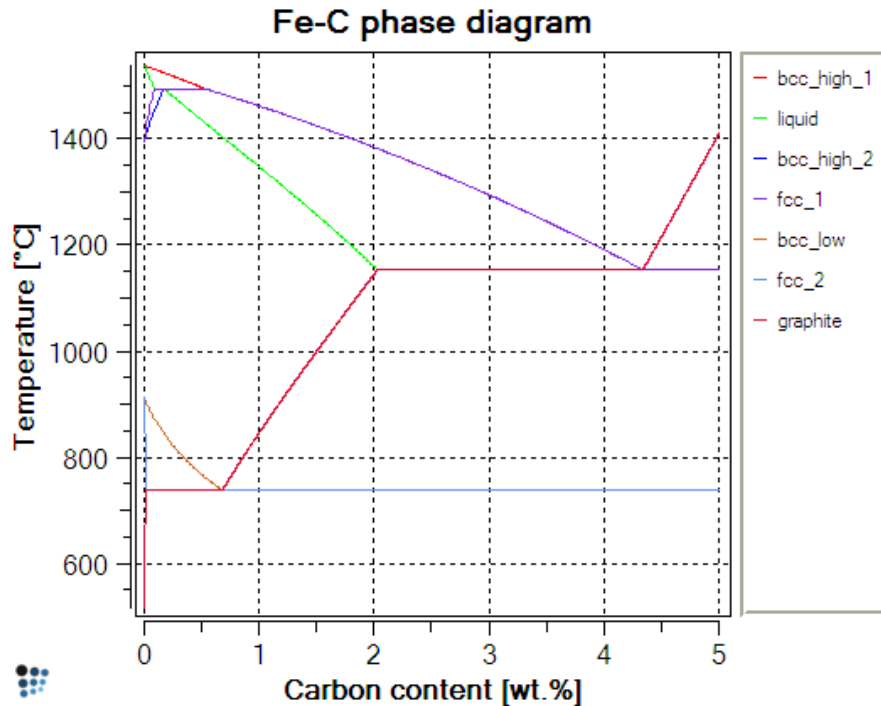
Fe-C phase diagram

SUGGESTED PARAMETERS FOR CALCULATION OF FE-C PHASE DIAGRAM

- **Upper boundary of high-T bcc**: Equilibrium at 1550°C (Tsol 'BCC_A2': 1533.98°C); step from 0 to 5 with interval of 0.01, max T-step 20

1. **Lower boundary of liquid**: Equilibrium at 1500°C (Tsol 'LIQUID': 1515.43°C); step with same parameters
2. **Lower boundary of high-T bcc**: Equilibrium at 1400°C (Tsol 'BCC_A2': 1429.60°C); same parameters
3. **Upper boundary of fcc**: Equilibrium at 1500°C (Tsol 'FCC_A1': 1460.18°C); same parameters
4. **Upper boundary of low-T bcc**: Equilibrium at 900°C (Tsol 'BCC_A2': 888.64°C); same parameters
5. **Lower boundary of fcc**: Equilibrium at 700°C (Tsol 'FCC_A1': 738.02°C). For this line, the parameters must be modified: decrease the interval to 0.001 or increase the T-step to 200. The latter solution (an interval of 0.01 and a T-step of 200) is acceptable because this boundary is a straight line so is correctly defined despite there being only a few points in this region. An error message (max no of iterations reached) may appear, but the line is calculated successfully.
6. **Upper boundary of graphite**: Equilibrium at 800°C (Tsol 'GRAPHITE': 738.02°C). In this case, the boundary is curved, so it is advisable to decrease the interval to 0.001 as well as increasing the T-step to 100 to obtain better resolution of the curvature. This boundary, like the cementite boundary discussed above, tends to 'overshoot' to very low temperature values. This can be prevented by setting the minimum carbon content for the stepped calculation to 0.0005 instead of 1e-9.

CONSECUTIVE ARTICLES

The tutorial is continued in article T9 - Calculating a pseudobinary phase diagram

T9: CALCULATING PSEUDOBINARY PHASE DIAGRAMS

This tutorial was tested on
MatCalc version 5.57 rel 0.057
license: free
database: mc_sample_fe.tdb

A pseudobinary phase diagram is an equilibrium diagram calculated for a ternary or higher-order system, in which the phase boundaries resulting from the variation of two of the element contents are calculated, while the amounts of all the other elements are kept constant.

CONTENTS:

- Further phase boundary calculations
- Coping with complex boundary shapes
- Diagrams with different reference elements

SETTING UP THE SYSTEM

Make a new workspace with the elements Fe, C and Nb and the phases FCC_A1, BCC_A2, LIQUID and CEMENTITE. Verify that Fe is selected as the reference element and enter the composition: 0.1 wt.% C, 0.3 wt.% Nb. Create a new p1-type plot window for the phase diagram.

FE-C PSEUDOBINARY WITH CONSTANT NB CONTENT

This is similar in many respects to the Fe-Fe$_3$C diagram calculated in Tutorial 8, but the presence of niobium stabilises an additional phase, FCC_A1#01 (which is essentially NbC). The stability of this phase has a strong dependence on both carbon and niobium contents. Only the low-carbon portion of the diagram, from 0 to 0.2 wt.%, is of interest in this tutorial. Begin, as in Tutorial 8, by calculating an equilibrium at 1550°C, then search for the BCC_A2 phase boundary. Step from 0 to 0.2 wt.% C, with an interval of 0.0005 and a maximum T-step of 20, tracing the BCC_A2 boundary. Drag and drop the T$C series into the plot and duplicate, lock and label it. Add the liquid and austenite (FCC_A1) upper boundaries and the lower boundary of the delta-ferrite (BCC_A2) to the diagram. Suggested equilibrium temperatures for finding these lines are as follows:

- LIQUID: 1450°C
- FCC_A1: 1500°C (N.B. the correct value of Tsol 'FCC_A1' should be 1483.41°C.)
- BCC_A2: 1450°C

The high-temperature part of the diagram should look like this:
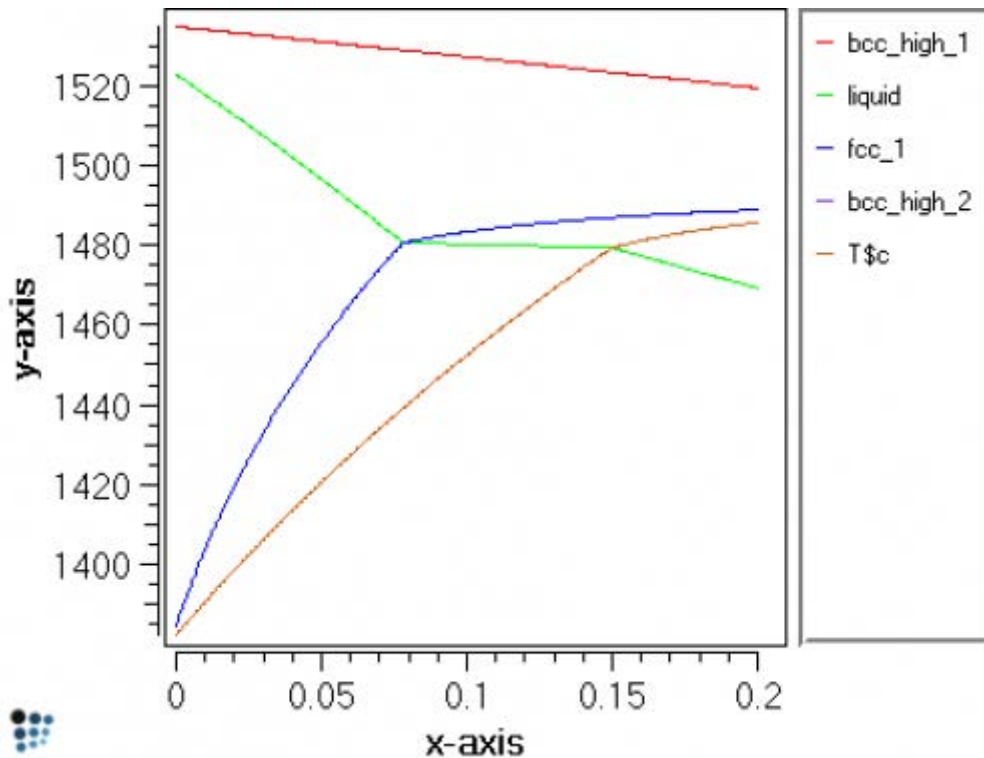
Next, calculate the boundary for niobium carbide (FCC_A1#01). The temperature of the boundary depends strongly on carbon content, but an equilibrium at 1450°C gives a suitable starting point for finding it.

Increase the maximum T-step to 100 to cope with the steepness of the curve. The boundary may extend to very small temperature values; in this case, change the scale on the y-axis to **'500..'** so that only the relevant information is shown.

The final three lines can be calculated as follows:

- Upper boundary of alpha-ferrite (BCC_A2): 900°C. The maximum T-step can be reduced again to 20.
- Lower boundary of austenite (FCC_A1): 700°C.
- Upper boundary of cementite 800°C. In case of error message (because of the steep boundary), set the maximum T-step to 100.

The finished diagram, with titles and labels added, should look like this:

Fe-C pseudobinary for 0.3 wt.% Nb
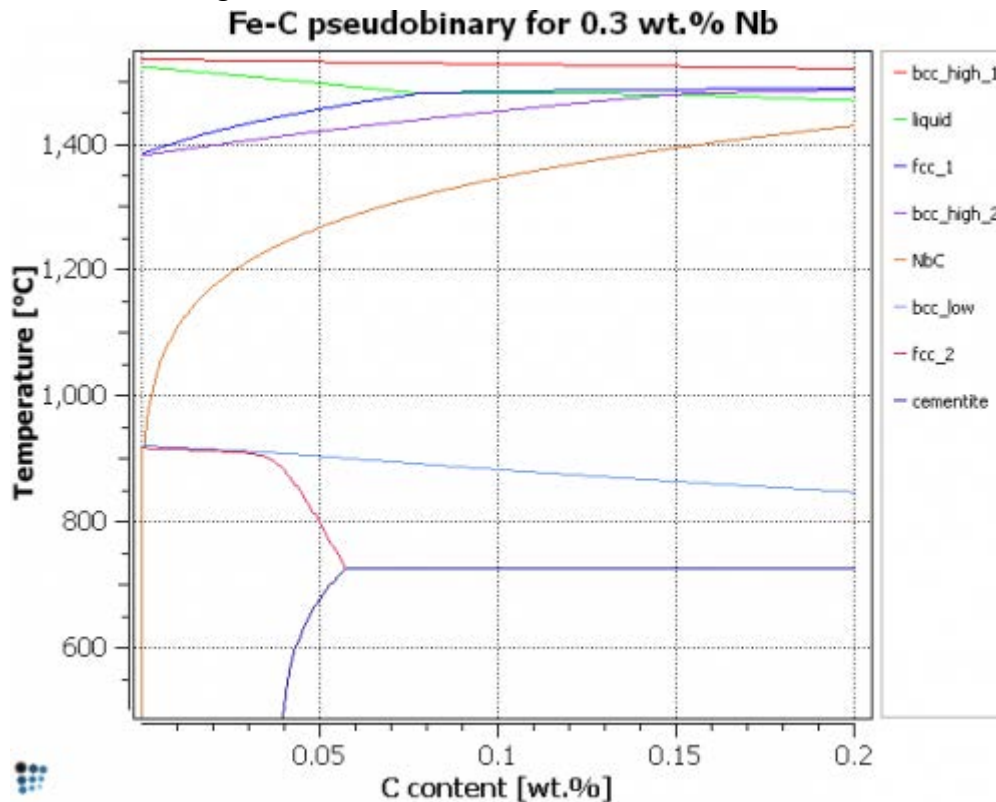
FE-NB PSEUDOBINARY WITH CONSTANT C CONTENT

In this case, the niobium content is to be varied from 0 to 1 wt.% for the stepped calculations. Proceed as before, by calculating an equilibrium at 1550°C and searching for the BCC_A2 phase boundary. For the stepped calculation, enter 0, 1 and 0.01 as the start, stop and interval values and under **'Boundary conditions'**, change the varying element to **'NB'** and **'max. T-step'** to **'20'**.

The boundaries can be calculated with the same starting equilibrium temperatures as for the Fe-C diagram, because the basis composition used for calculating the equilibrium and finding a point on the boundary remains the same (0.1 wt.% C, 0.3 wt.% Nb). Search for and plot all the following boundaries:

- Upper boundary of delta-ferrite (BCC_A2)
- Lower boundary of liquid
- Upper boundary of austenite (FCC_A1)
- Lower boundary of delta-ferrite
- Upper boundary of alpha-ferrite (BCC_A2)
- Lower boundary of austenite
- Upper boundary of cementite (may need modification of maximum T-step to 100-200)

The NbC (FCC_A1#01) boundary is slightly more complex in this example, so it will be considered in more detail. Firstly, calculate an equilibrium at 750°C and search for the FCC_A1#01 phase boundary varying niobium content. This is at 4.44e-5 wt.% Nb. Make a

stepped calculation from 0 to 1 wt.% Nb as usual. Part-way through this calculation, the following message is displayed:

The calculation starts at the niobium content used to calculate the equilibrium (0.3 wt.%), and this is first increased up to the **'stop'** value (1 wt.%, in this case) and then decreased to the **'start'** value (0). The message above implies that the calculation cannot proceed any further in the increasing-Nb direction. Click on 'Yes' to calculate the decreasing-Nb part of the boundary. It can be seen that the NbC curve terminates at the **'cementite'** line. Also in the larger Nb content range, the curve is cut at a niobium content of around 0.57 wt.%.

In order to find the phase boundary outside these limits, additional calculations must be performed. Dealing with the NbC phase boundary below the **'cementite'** line is quite straightforward. After locking the previous curve, calculate an equilibrium at 500°C and search for the FCC_A1#01 phase boundary at this temperature. Due to the steep boundary, it is recommended to set the calculation step to 0.001 and the max. T-step value to 200. The final part of the NbC boundary (above the **'liquid'** line) is plotted after setting the Nb content to 0.7 wt. %, calculating equilibrium for 1000°C and finding the phase boundary for this alloy composition (at 1466.78°C) - perform a step calculation with the step of 0.01 and max. T-step of 20. The finished diagram is shown below.

Fe-Nb pseudobinary for 0.1 wt.% C
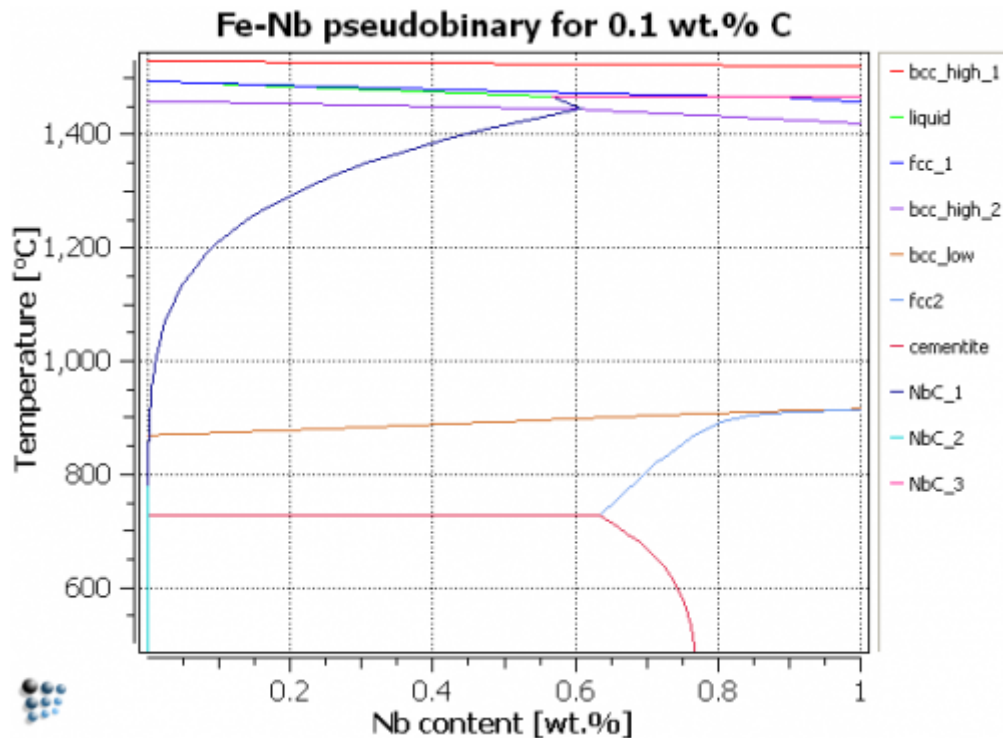
NB-C PSEUDOBINARY WITH CONSTANT FE CONTENT

The final part of this tutorial considers the effect of both C and Nb contents on the stability of NbC. Previously, iron has been set as the **'reference element'**; this means that when the amount of the varying species increases, the amount of iron in the system decreases so that the total composition sums to unity. For the Nb-C pseudobinary, niobium will instead be set as the reference element, and a fixed iron content will be imposed, so that the sum of niobium content and carbon content is constant. In addition, the element contents will be expressed in mole fractions, so that the effect of Nb:C ratio on carbide stability can be investigated. Open **'Global > Composition'** and switch to **'mole fraction'**. Change the reference element from Fe to Nb. Enter the compositions 0.995 Fe, 0.004 C.

As usual, search for the upper boundary of the delta-ferrite phase. This should be found at 1529.63°C. In the stepped calculation dialogue box, enter 0, 0.005 and 1e-5 as the start, stop and interval values. Set the varying element to **'C'** and the maximum T-step to 20. In the **'Options'** section on the right-hand side of the box, remove the selection mark by the side of 'Composition in weight percent' so that it will instead be in mole fraction. Calculate the following lines. The solution temperatures are given as a guide, as well as notes on calculation settings.

- BCC_A2: 1529.63°C
- LIQUID: 1486.84°C. A warning message may appear; accept this with 'Yes'.
- FCC_A1: 1487.04°C. The same warning may appear.
- BCC_A2: 1447.56°C
- BCC_A2: 882.04°C. Step from 0 to 0.00498 rather than 0.005 to avoid convergence problems.
- FCC_A1: 726.62°C. Step from 0 to 0.00498.
- CEMENTITE: 726.62°C

Finally, the line for FCC_A1#01 can be calculated. Search for this line, which should be found at 1255.80°C. The temperature of this phase boundary decreases very steeply at both extremities of the x-axis, because the phase becomes less and less stable as either the niobium content or the carbon content tends to zero. To obtain an idea of the shape of the curve, set the start and stop-values as 0.0001 to 0.0049 (A maximum T-step of 20 is OK for this calculation.) Modifications can then be made to the calculation parameters, decreasing the start value, increasing the stop-value and increasing the maximum T-step to try to extend the curve further towards the edges.

The finished diagram should look like this:
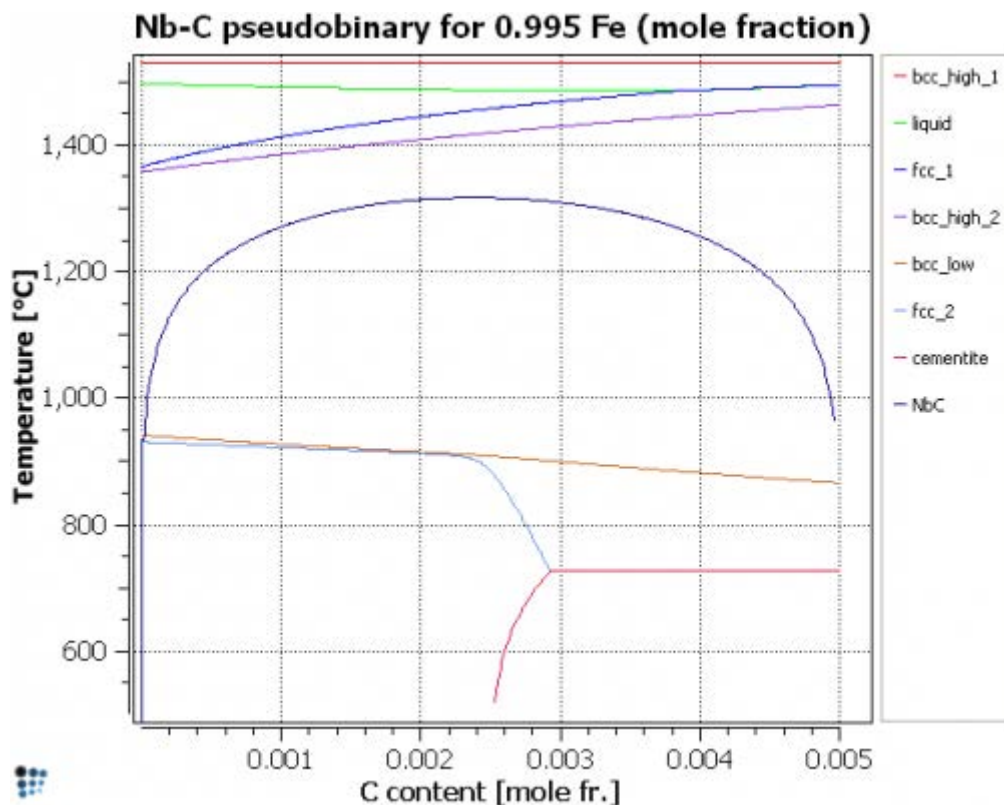
CONSECUTIVE ARTICLES

The tutorial is continued in article T10 - T0- temperature in Fe-Cr-C

T10: T_0-TEMPERATURE IN FE-CR-C

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb

CONTENTS:

- T_0- temperature calculation
- Martensite / Bainite transformation
- Variation of T_0- temperature with carbon and chromium content
- Import and display of experimental data into plots

The **T_0-temperature** is defined as the temperature where two phases of identical chemical composition have the same molar Gibbs free energy. This temperature is an important quantity in the field of **diffusionless phase transformations**, i.e. the bainitic and martensitic transformation. In the present example, we will discuss some thermodynamic aspects of the austenite/martensite transformation and apply T_0-temperature calculations to the evaluation of transformation temperatures.

## STEP 1: DEFINE THE THERMODYNAMIC SYSTEM (SEE ALSO TUTORIAL T2)

Create a new workspace file. From a suitable database (mc_sample_fe.tdb) define the elements **Fe**, **Cr** and **C** as well as the phases **BCC_A2** (ferrite) and **FCC_A1** (austenite). Enter the system composition with **wp(C) = 0.1** and **wp(Cr)=1.0**. Set initial values with **'Calc - Set start values'** or **Ctrl+Shift+F**. Calculate an equilibrium at **800°C**.

STEP 2: CALCULATE THE T_0-TEMPERATURE

Before evaluation of the T_0-temperature, an equilibrium located in the **one-phase region** of the parent phase must be calculated in order **to set the composition of one of the phases equal to the system composition**. The parent phase is austenite so the solubility temperature of BCC_A2 will be evaluated with **'Calc - Search phase boundary…'** or **Ctrl+Shift+T**. As a result, MatCalc displays in the **'Output'**window

`Tsol 'BCC_A2': 856,87 C (1130,03 K) iter: 5, time used: 0,03 s`

In the **'Phase summary'** and **'Phase details'** window, only the FCC_A1 phase is denoted as active (mole fracton = 1). We can now proceed with this initial condition. For convenience, store this (current) state in a calculation state with the name **'Start austenite'** by selecting **'Global - CalcStates - Create…'**.
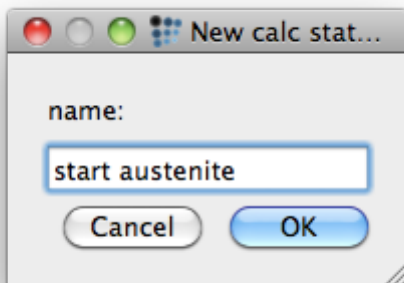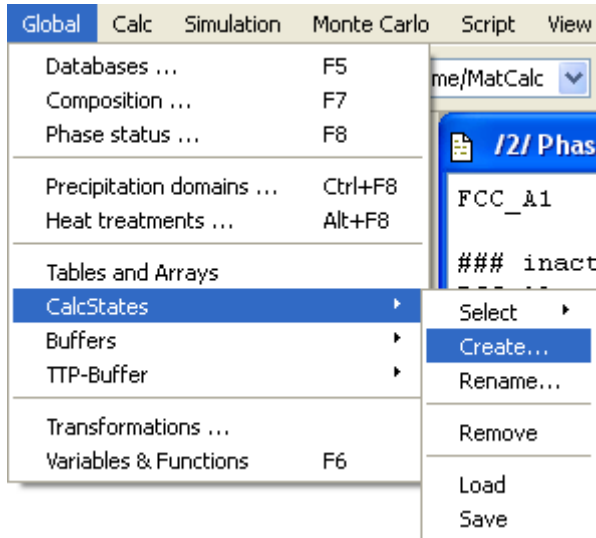
We can now evaluate the T_0-temperature for austenite and ferrite with **'Calc - Search phase boundary…'** or **Ctrl+Shift+T**. The following, well-known, dialog box appears:
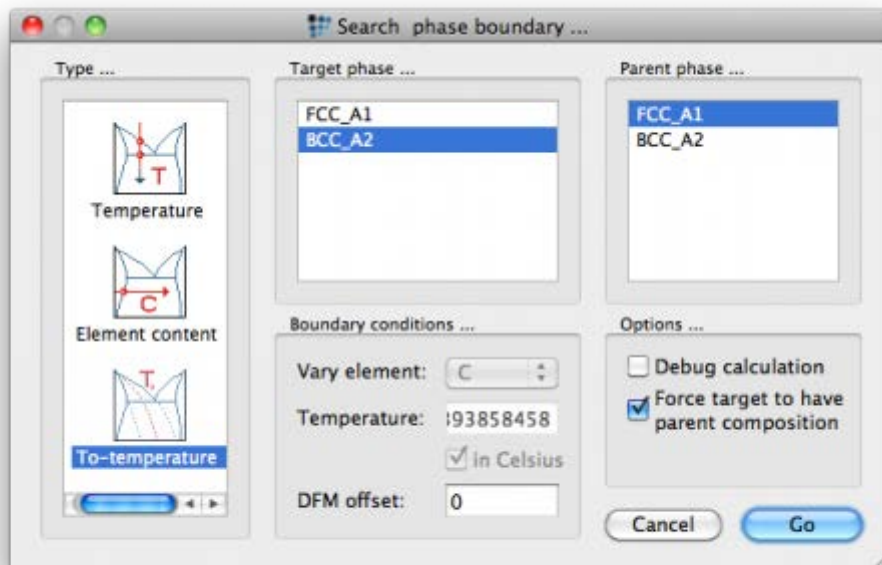
Select **'T_0-temperature'** in the type listbox, **'BCC_A2'** as target phase and **'FCC_A1'** as parent phase. The check box **'Force target to parent composition'** must be chosen, because the

composition of BCC_A2 wil be adjusted according to the parent composition. The energy difference (**DFM offset**) can be left as default (zero). Press **'Go'** to start the calculation. The result is shown below

```
T0(FCC_A1/BCC_A2): 793,394 C (1066,55 K)
iter: 2, time used: 0,05 s
- OK -
```

The phase details window shows:

```
#### /FCC_A1/ moles: 1, gm: -47047.2 (-47047.2), sff: 0.995371
Phasestatus: entered - active
FE +9.84677e-001 CR +1.06937e-002 C +4.62933e-003

### inactive ###

#### /BCC_A2/ moles: 0, gm: -47047.2 (-47047.2), sff: 0.995371
Phasestatus: entered - not active (dfm=3.412e-009)
FE +9.84677e-001 CR +1.06937e-002 C +4.62933e-003
```

It is obvious that, at the temperature of 793.394°C, FCC_A1 and BCC_A2 of the same composition have the same molar Gibbs free energy of gm=47047.2 J/mole.

STEP 3: EVALUATE T_0- TEMPERATURE AS A FUNCTION OF CHROMIUM CONTENT

Let us now investigate how the T_0- temperature for ferrite and austenite varies with the chromium content. From the menu select **'Calc - Stepped calculation…'** or press **Ctrl+T**. In the left listbox of the **'Step equilibrium …'** window, select type **'T_0 temperature'**. Select **'FCC_A1'** for the parent phase and **'BCC_A2'** for the target phase. Don't forget to select chromium as the independent element. Enter the chromium range between **'0'** and **'10'** weight percent in steps of **'0.5'** and don't forget to mark the **'Force identical composition'** box. The **'Step equilibrium …'** window looks now as follows.
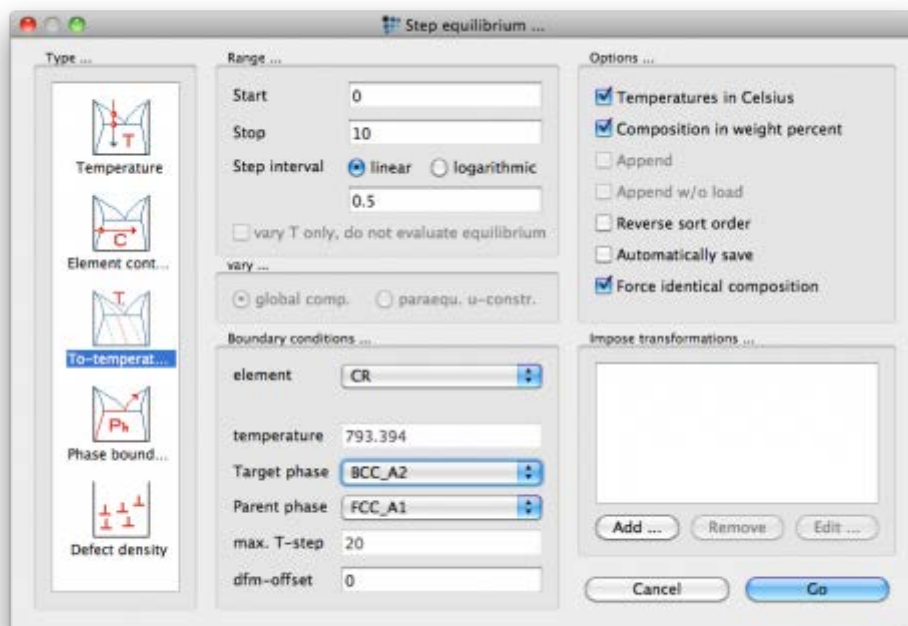
Press **'Go'** to start the calculation. The result can be displayed in the well known **'XY-data'** plot. Create the plot and drag and drop the **T$c** variable from the variables window into the plot. Edit the **'x-axis'**, **'y-axis'** and **'legend'** (see also Tutorial 4 or Tutorial 5) such that the result of the stepped T_0- temperature calculation looks as follows.
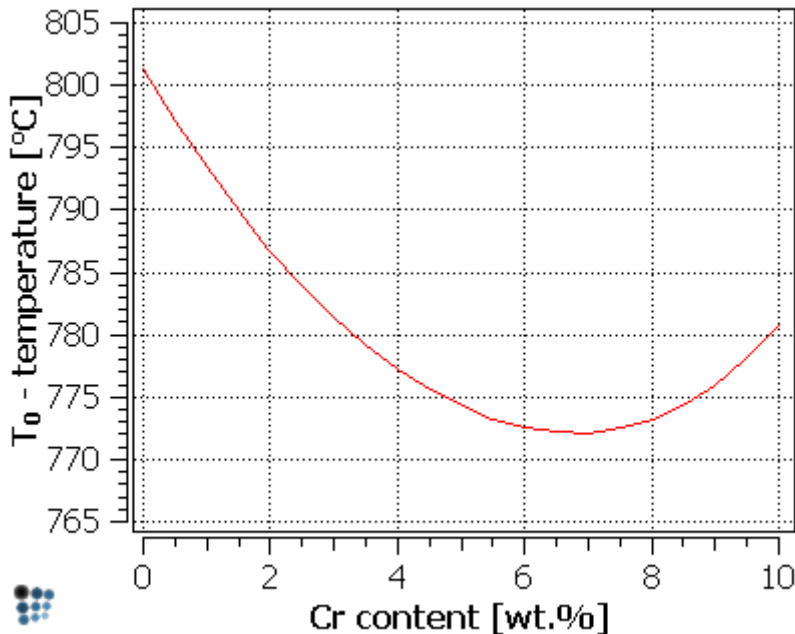

STEP 4: EVALUATE T_0-TEMPERATURE AS A FUNCTION OF CARBON CONTENT

In the same way, similar to the evaluation of the dependence of the T_0- temperature on the chromium content, it is possible to calculate the T_0- temperature as a function of the carbon content. Therefore, rename the **'_default_'** buffer selecting **'Global - Buffers - Rename …'** and give it the name **T_0- chromium**. Then create a new buffer (**'Global > Buffers > Create …'**) with the name **T_0- carbon** and load the calculation state **'Start austenite'** (make sure that the current buffer is the **'T_0- carbon'** - buffer). Analogously to the calculation before, carry out a stepped calculation. Press **'Calc - Stepped calculation …'** or press **Ctrl+T**, enter the following settings and press **'Go'**.
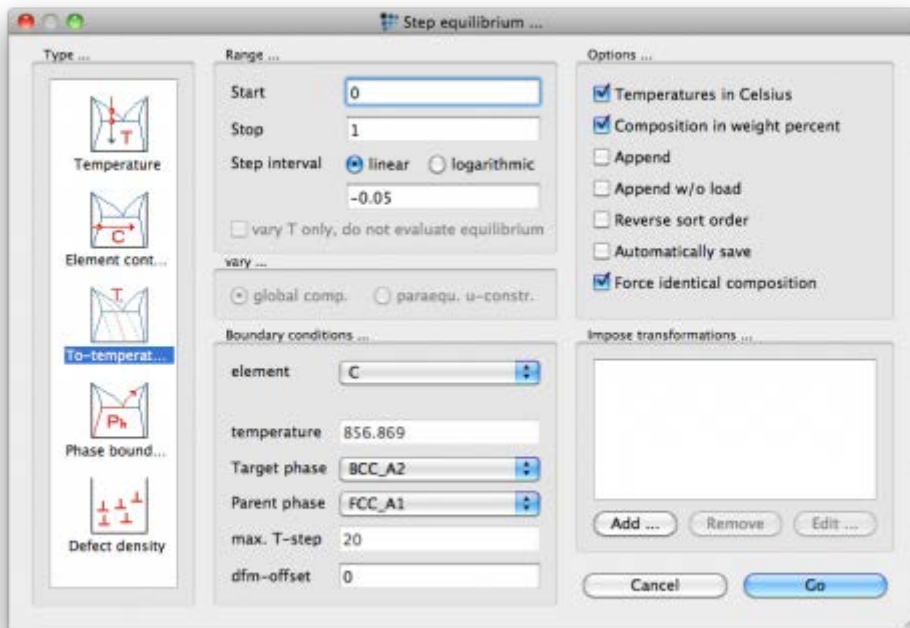
The graph for the T_0- temperature dependence for varying carbon content should look like the figure below. **There is no need to create a new plot**. The T_0- temperature line in the figure can be simply changed by **switching** from **'T_0 - chromium'** buffer to the **'T_0- carbon'** buffer **in the options window**.
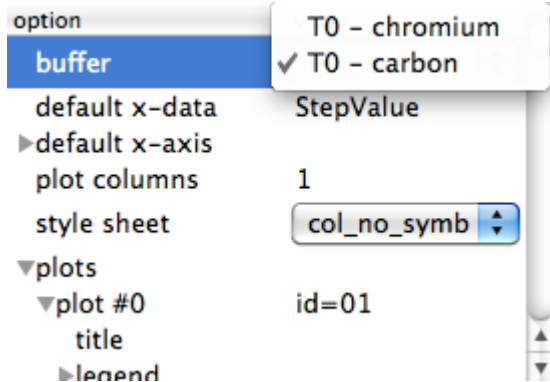
Afterwards, the x- and y-axes must be rescaled and in the case of the x-axis renamed. So the result looks as follows.
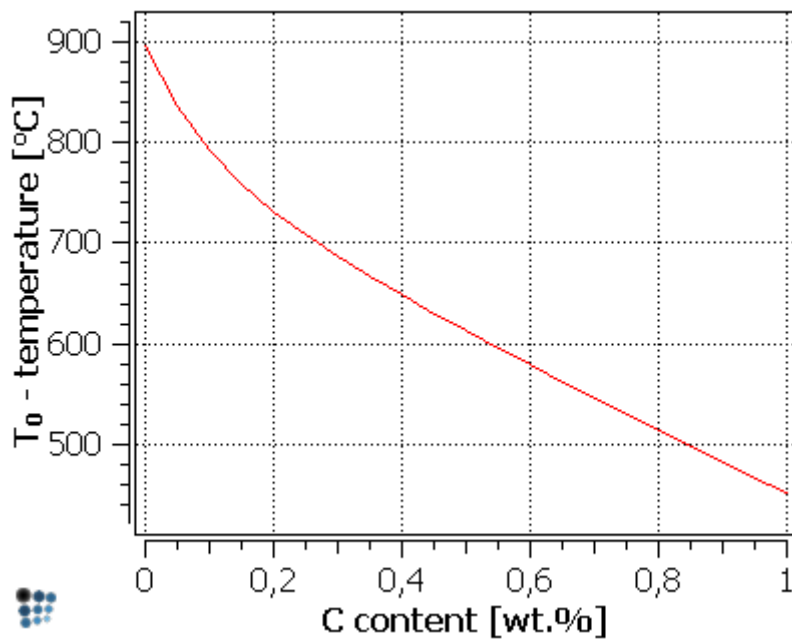
The strong dependence of the T_0- temperature on the carbon content is evident. This is reflected in the strong influence of carbon on the martensite start temperature.
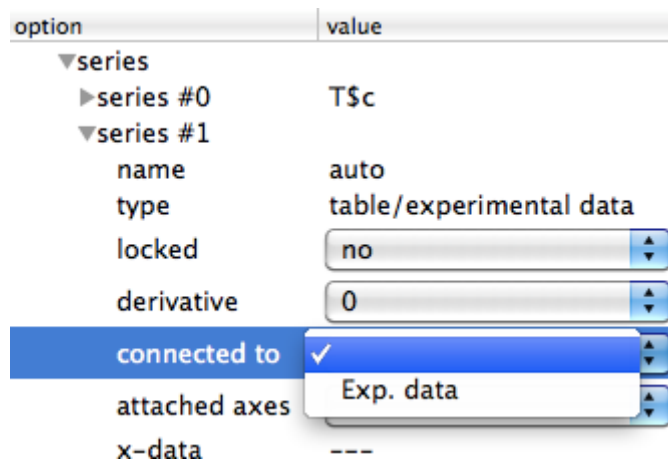
STEP 5: ADD SOME EXPERIMENTAL DATA ON MARTENSITE START TEMPERATURES

The experimental data, which will be added to the recent plot, are taken from ref. [1]. Before doing so, we must create a new buffer. So, none of the former results will be lost. Name the new buffer as **'T_0 with offset'** (further calculations with various dfm-offsets will be done …) and create a table selecting **'Global - Tables and arrays …'**. Press **'New …'** and call the table **'Exp. data'**. After selecting **'Edit …'**, enter the following measured martensite start temperatures into the table or copy them from a file (the file is here).

Carbon content[wt%]	Martensite start temperature
0	540
0.086	510
0.1936	475
0.2409	480
0.2495	470
0.2581	440
0.3011	430
0.3226	410
0.3871	410
0.3871	400
0.3871	395
0.4560	405
0.4947	355
0.5054	375

0.6022	330
0.6022	320
0.7097	280
0.7312	280
0.7743	265
0.8173	240
0.8603	225

Press **'OK'** twice and insert the experimental data into the plot as a new series (right-click in **'options'** window and select **'New series > table experimental data'**) and switch to **'Exp. data'** in **'connected to'** box (see also Tutorial 5).

option	value
▼series	
▶series #0	T$c
▼series #1	
name	auto
type	table/experimental data
locked	no
derivative	0
connected to	✓
	Exp. data
attached axes	
x–data	---

Rescale the y-axis (set scaling as **'auto'**) and edit the legend and the series names. The result looks as follows.
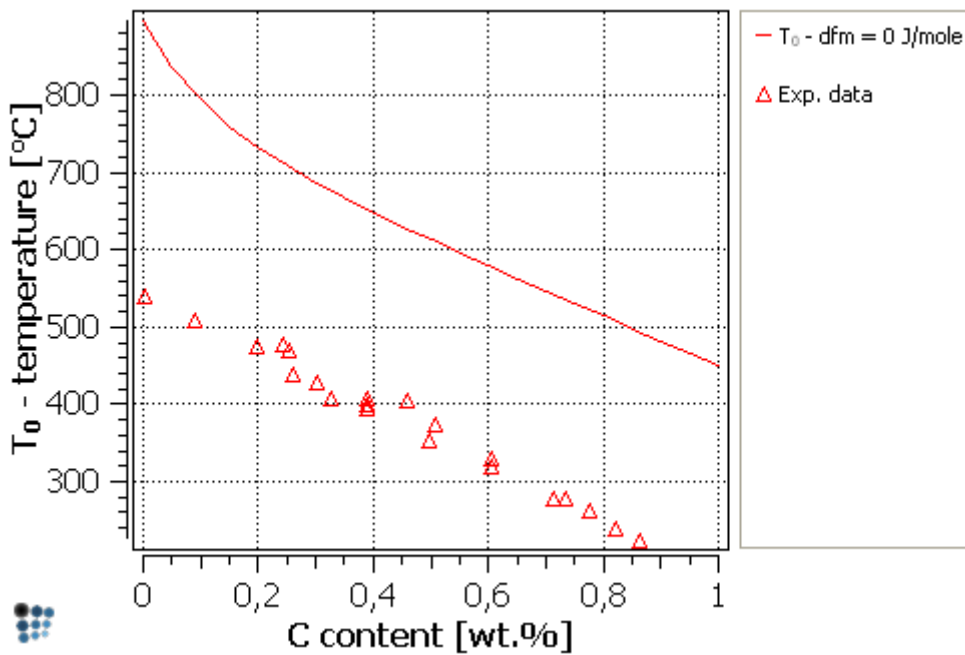

Apparently, the calculated T_0- temperature does not fit the experimental data, however the curve runs parallel to it with the calculated temperatures being higher. The reason is that a certain amount of driving force is required to start the martensite transformation. This extra

energy, or extra driving force, is of the order of 1.2 to 2.5 kJ/mol (depending on the composition of the alloy) and can be defined in the field **dfm-offset**. Default value for this parameter is zero.

To evaluate how high this extra energy is as a function of carbon content, stepped calculations with different dfm-offsets can be performed. Carry out two simulations, one as a steped T_0- temperature calculation with a **dfm-offset** of **1200 J/mole** and one with **1700 J/mole**. Before starting lock the first series (T_0- dfm=0 J/mole). So the first graph will be conserved for further comparison.

Select **'Calc - Stepped calculation …'** and complete the dialog box as follows:
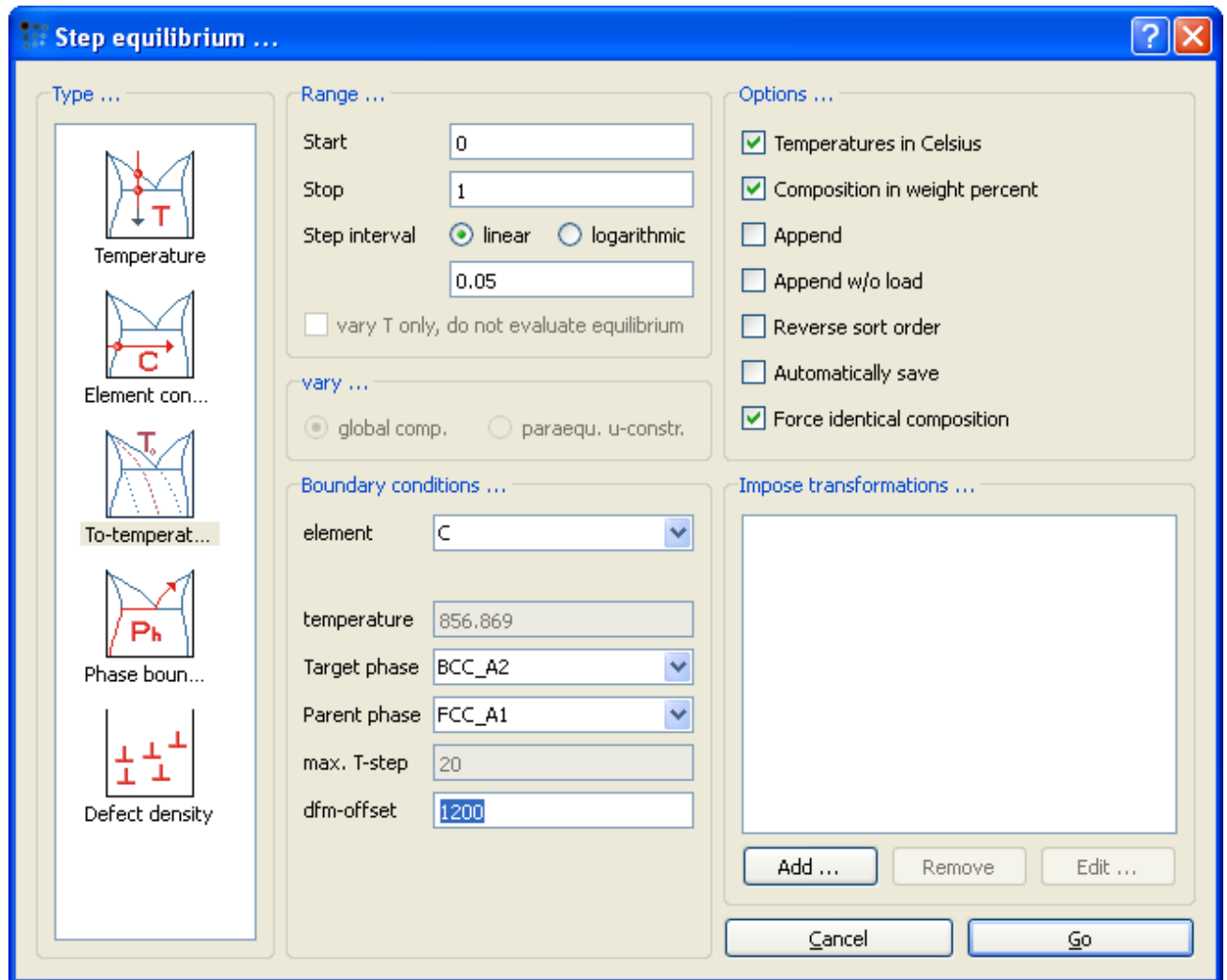
Drag and drop the **'T$c'** variable again into the plot and rename the series to **T₀ - dfm=1200 J/mole**. Do the same for a dfm-offset of 1700 J/mole.

The plot now looks like follows.
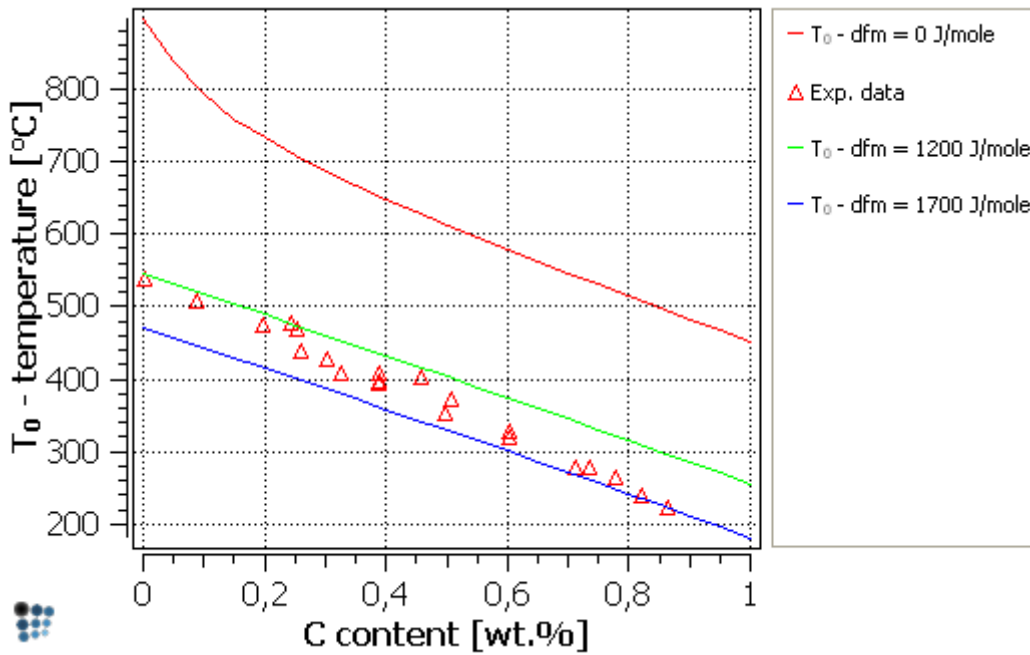
A dfm-offset in the range of 1200-1700 J/mole can be used to obtain reasonable agreement between the calculations and the experimental data.

CONSECUTIVE ARTICLES

The tutorial is continued in article T11 - Simulation of solidification of 0.7C 3Mn steel

[1)]**References**

[1] Z. Jicheng and J. Zhanpeng, Acta met. mater. 38 (1990) 425-431.

T11: Simulation of solidification of 0.7C 3Mn steel

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb

Contents:

- Scheil calculation
- Back-Diffusion
- Composition set
- Solid-solid transformation

The **Scheil-Gulliver method** allows calculating the **fraction and composition of all phases during solidification** step by step from the liquidus temperature to the temperature where solidification of the residual liquid phase occurs [1]. The particular residual fraction at final solidification is dependent on the cooling rate. Generally, the fraction is higher, the higher the cooling rate is. At slow cooling rates, the liquid film can become very thin and the residual liquid enriches more than in the case of higher fraction residual liquid at solidification.

According to the Scheil-Gulliver hypothesis, illustrated in the figure below (Fig.1), a solidifying liquid with the initial composition C_0 is slightly undercooled. Consequently, a certain fraction of solid is formed with a composition of $C_{S,1}$ with the remaining liquid phase with the composition $C_{L,1}$. Both phases are in **local equilibrium following the lever rule**. From that instant on, the composition of the solid phase with regard to the substitutional atoms is frozen due to the Scheil-Gulliver assumption of very slow (and therefore negligible) diffusion in the solid phase. The interstitial elements boron, carbon and nitrogen are assumed to be nevertheless highly mobile in the liquid phase as well as the solid phase. Therefore, these elements are assumed to be able to establish equilibrium between the liquid and solid phases due to back-diffusion of enriched solute atoms from the liquid phase into the solid phase. This process occurs repeatedly, enriching the solid phase as well as the liquid phase with solute during cooling (Fig.1:$C_{L,i}$ and $C_{S,i}$).
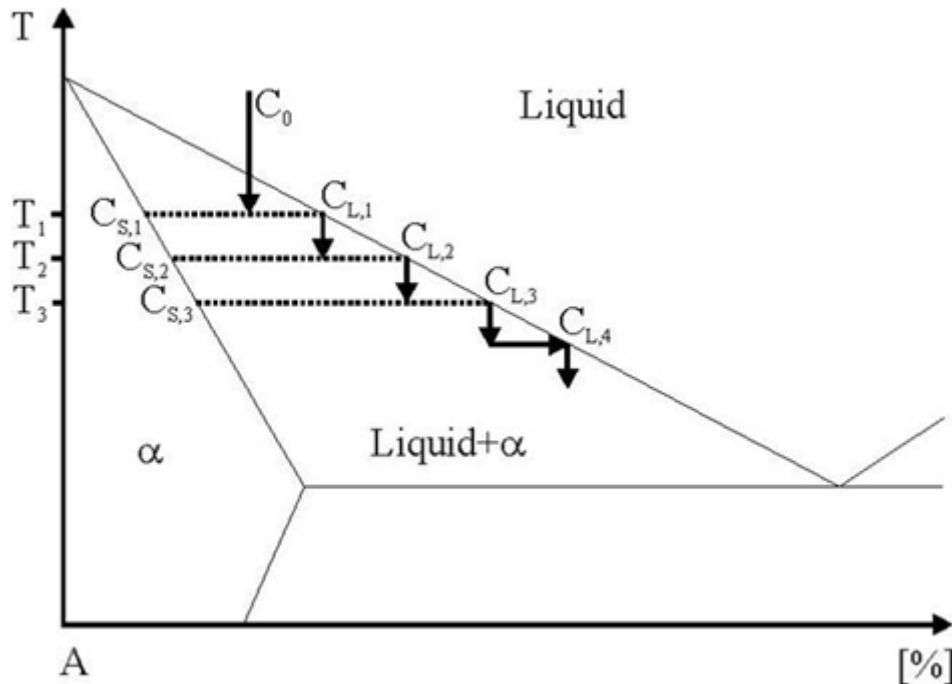
Fig.1: Scheme of Scheil solidification of a hypothetic Fe-C alloy. During solidification the actual liquid phase, beginning with C0, is undercooled and solidifies according to the lever rule enriching the liquid phase with solute atoms

When solidification is finished, the microstructure of the solid phase shows a composition gradient from the regions where the solidification started (centre of the dendrite) to the areas where the last liquid solidified (outer shell of the dendrite). The composition of the residual liquid at final solidification corresponds to the composition of the interdendritic regions. It should be noted that the Scheil-Gulliver analysis yields an upper limit of segregation since the substitutional elements also have a finite mobility and have some potential of back-diffusion.

Scheil-type calculations in multi-component systems have proven to be a useful method to simulate solidification processes. The present example shows how to carry out this type of simulation with MatCalc and demonstrates the effect of carbon back-diffusion on the solidification process. Moreover, the influence of solid-solid phase transformations, i.e. the peritectic transformation, is analyzed.

STEP 1: SETUP THE THERMODYNAMIC SYSTEM (SEE ALSO TUTORIAL T2)

Create a new workspace file. From a suitable database (mc_sample_fe.tdb) define the elements **Fe**, **Mn** and **C** and the phases **liquid**, **BCC_A2** (ferrite), **FCC_A1** (austenite) and **Cementite**.
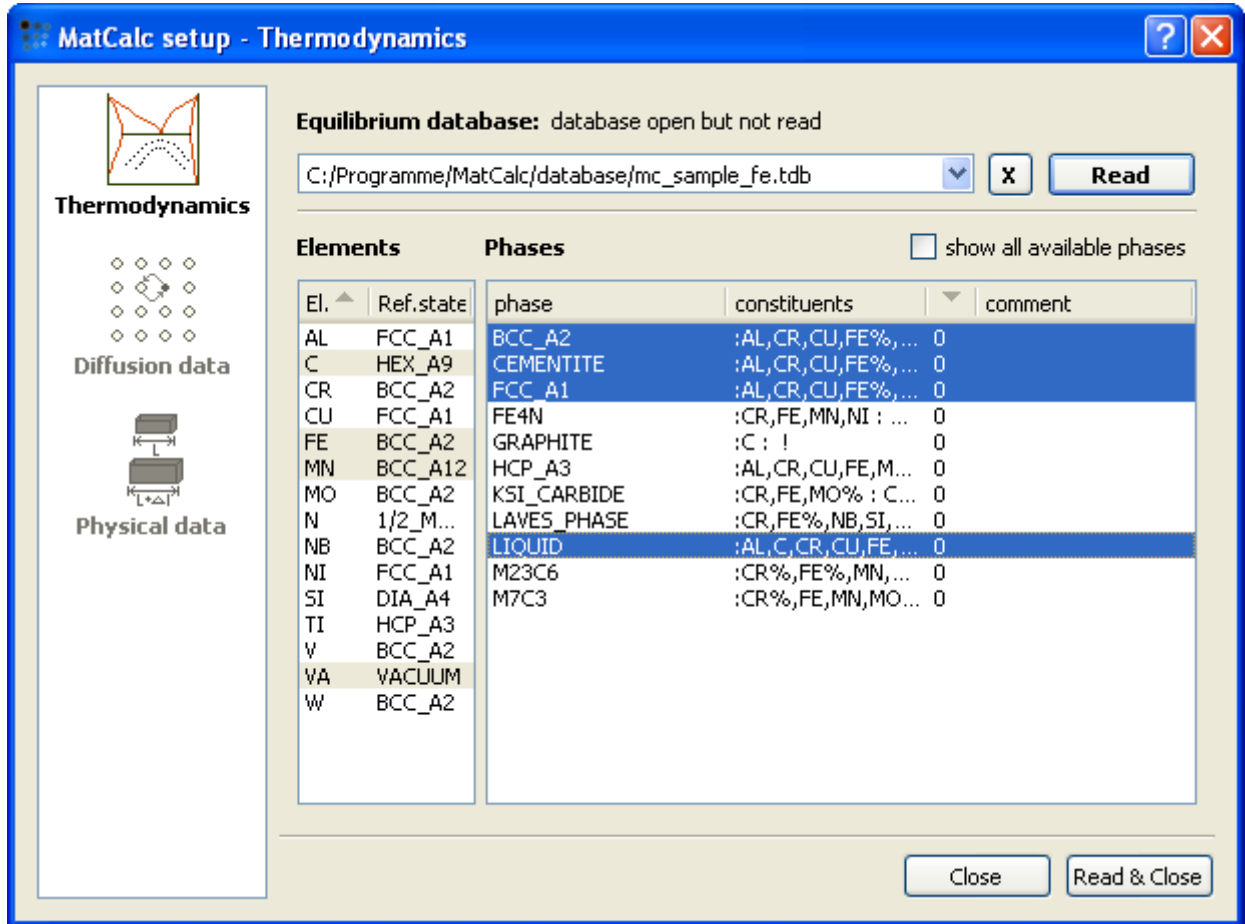
Enter the system composition in weight percent as listed in the subsequent figure selecting **'Global Composition …'** or pressing the **F7** key.
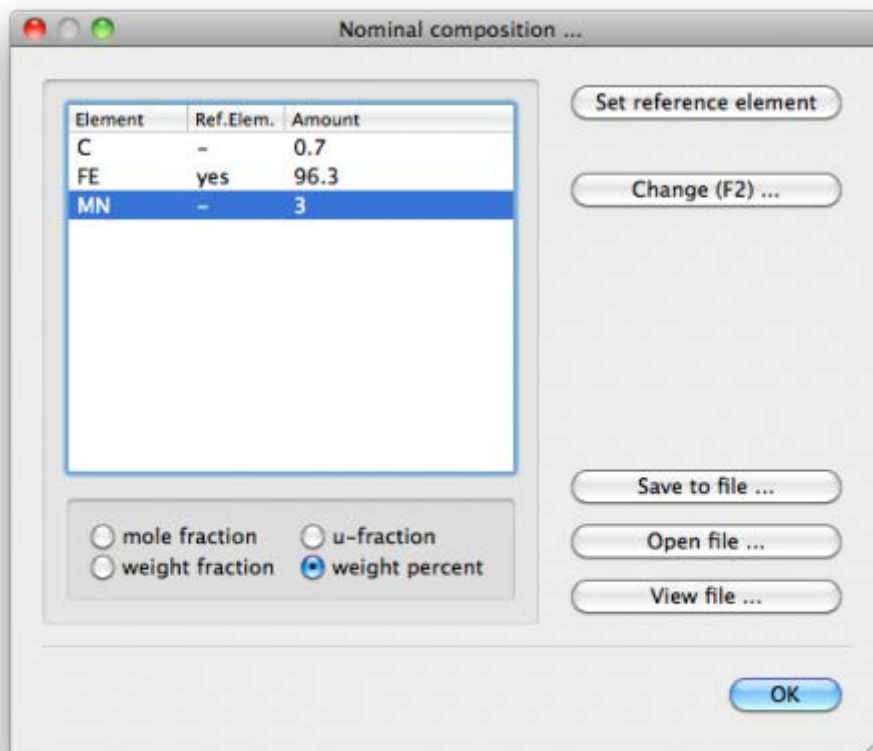
Set initial values with **'Equilibrium-Set start values'** or **Ctrl+Shift+F**. Calculate equilibrium at 1600°C. The results in the **'Phase summary'** window are

```
LIQUID  *              act    1,00000e+000 dfm: +0,00000e+000
### inactive ###
BCC_A2                 - OK -  0,00000e+000 dfm: -1,02442e+003
FCC_A1                 - OK -  0,00000e+000 dfm: -1,08259e+003
CEMENTITE              - OK -  0,00000e+000 dfm: -1,27829e+004
```

STEP 2: CARRY OUT A SCHEIL CALCULATION

Since we expect austenite to be the first phase to form on solidification, let us first look for the solubility temperature of this phase. Select **'Calc - Search phase boundary …'** or press **Ctrl+Shift+T** and select **FCC_A1** as target phase.
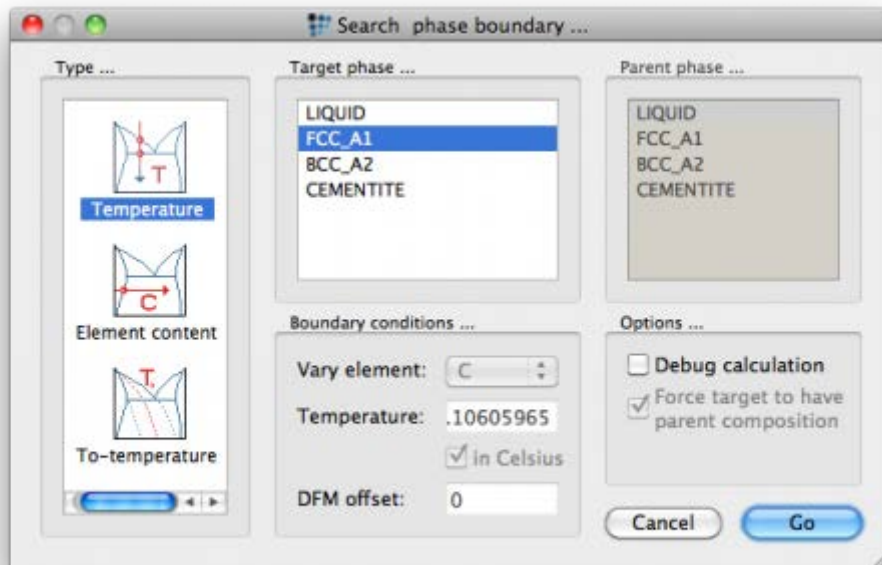
Press **'Go'**:

`Tsol 'FCC_A1': 1471,11 C (1744,27 K) iter: 4, time used: 0,03 s`

The first solid phase becomes stable at **1471.11°C**. So let us start with the Scheil simulation at **1500°C** and go down to **1000°C** in steps of **10**. Open the Scheil-calculation dialog with **'Calc - Scheil calculation …'** or press **Ctrl+H**.
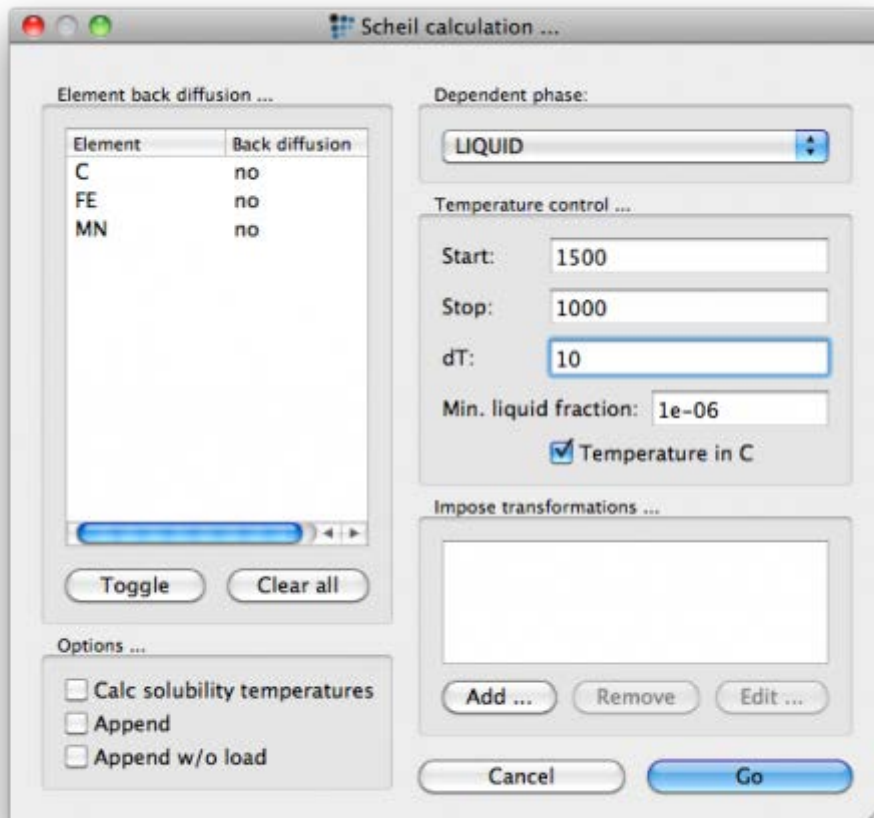
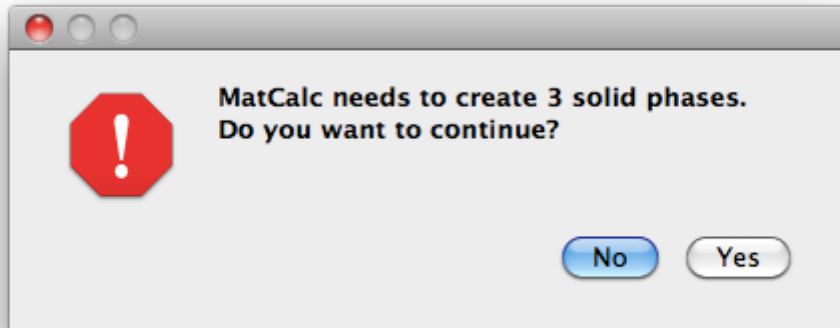Press **'Go'** to start the simulation. In order to be able to remove the equilibrium content of solid phases from the system after each temperature step, MatCalc needs to create **copies of all phases except the dependent** (liquid) **phase**. MatCalc therefore asks


Click **'Yes'**. MatCalc then creates 3 new phases with the name of the original phase plus the suffix **'_S'**. This suffix denotes that the corresponding phase is a **'solid'** phase. The result in the **'Output'** window looks as follows

```
Checking solid phases ...creating phases: ...- OK -
- OK -
Searching initial equilibrium ...
1, 1.02 s, 1500.00 C (1773.16 K), its 2, f=1.00000000, LIQUID
...
3, 1.03 s, 1480.00 C (1753.16 K), its 2, f=1.00000000, LIQUID
4, 1.05 s, 1470.00 C (1743.16 K), its 5, f=0.96983965, LIQUID FCC_A1
...
12, 1.13 s, 1390.00 C (1663.16 K), its 6, f=0.25223994, LIQUID FCC_A1
13, 1.14 s, 1380.00 C (1653.16 K), its 6, f=0.22786341, LIQUID FCC_A1
14, 1.16 s, 1370.00 C (1643.16 K), its 6, f=0.20736906, LIQUID FCC_A1
15, 1.16 s, 1360.00 C (1633.16 K), its 6, f=0.18993222, LIQUID FCC_A1
...
39, 1.41 s, 1120.00 C (1393.16 K), its 5, f=0.05684065, LIQUID FCC_A1
40, 1.42 s, 1110.00 C (1383.16 K), its 11, f=0.00000000, FCC_A1 CEMENTITE
fraction of phase 'LIQUID' smaller than 1e-006. Calc finished
Steps: 41, CalcTime: 2.67 s
AktStepVal: 1383.160000
- OK -
```

The current value of the fraction liquid at each temperature step is displayed with **'f=xxx'** in each line. The final eutectic is reached at T=1110°C. When the fraction liquid comes **below 1e-6 (minimum liquid fraction)** , the dependent phase is dissolved and the calculation is finished. Let's now look at the result.

Create a **XY-data** plot that shows the fraction of residual liquid as a function of temperature. The correct variable is **F$LIQUID**, you have to change the default x-data to **T$C** in the options window to show °C instead of K. Rescale the **x-axis** from **1100°C to 1500°C**. A few other settings were made until the result looks as follows
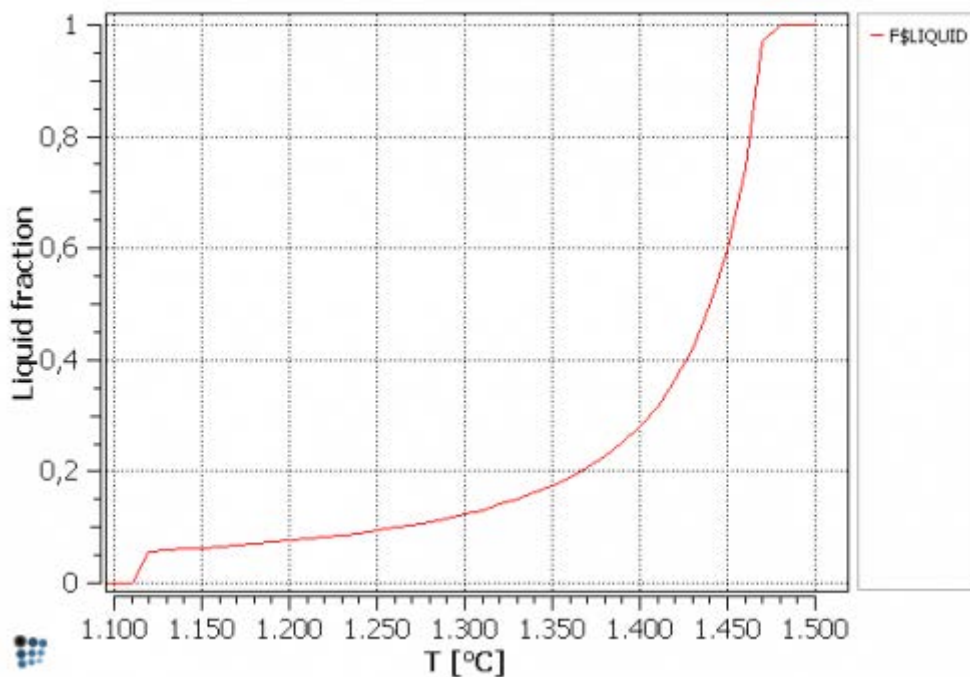
STEP 3: ADD A SCHEIL CALCULATION WITH BACK-DIFFUSION OF CARBON

The solidification of the current steel as calculated by the Scheil model predicts final solidification at too low temperature. In reality, **carbon atoms are fast enough** not only in the liquid but also in the solid to be able **to equilibrate between the solid and liquid phases**. Therefore, to get more realistic simulation results, we must allow for **back-diffusion of carbon**. First, in order not to loose the results of the previous simulation, rename the current buffer to **'Scheil'** and create a new one with the name **'Scheil with BD of C'**. Open the Scheil calculation dialog with **'Calc - Scheil calculation …'** or press **Ctrl+H**. Highlight carbon in the list box and press **'Toggle'**.
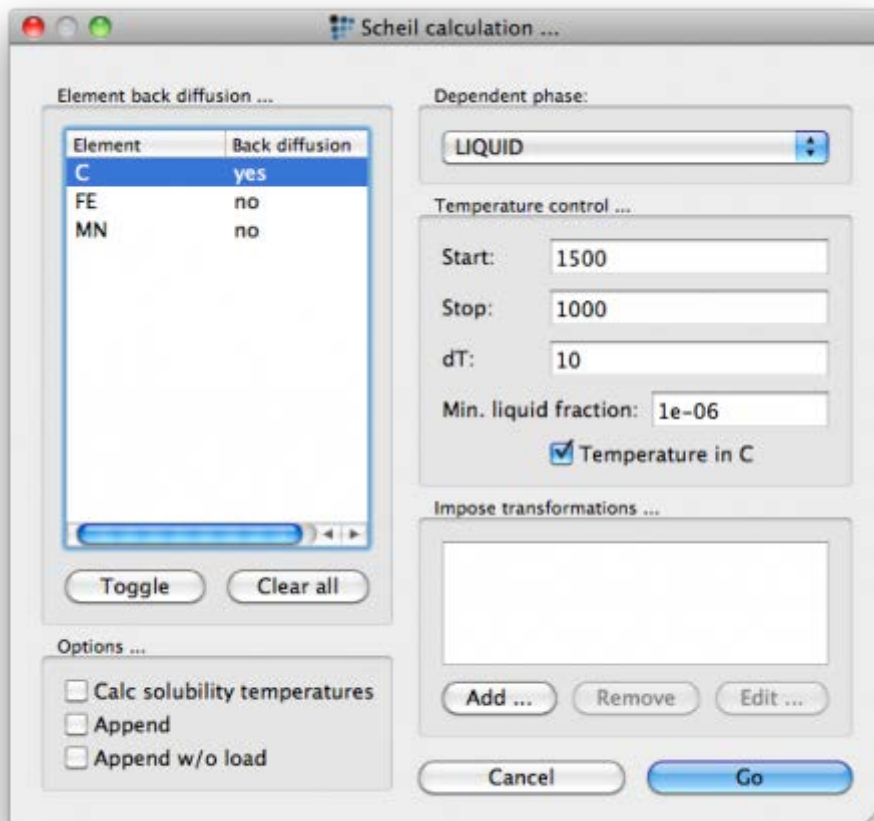
Press **'Go'** to start the simulation. After each temperature step, MatCalc sets up a paraequilibrium calculation, where all elements without back-diffusion have fixed composition variables and **only the elements with back-diffusion are unconstrained**. By that means, carbon is always brought back into equilibrium with regard to the **solid and liquid** phases after a regular Scheil simulation step is carried out.

We are going to display the Scheil curve with and without back-diffusion in one window. Therefore, first, lock the previous Scheil calculation, which is still displayed in the diagram window and name it **'Scheil'**.
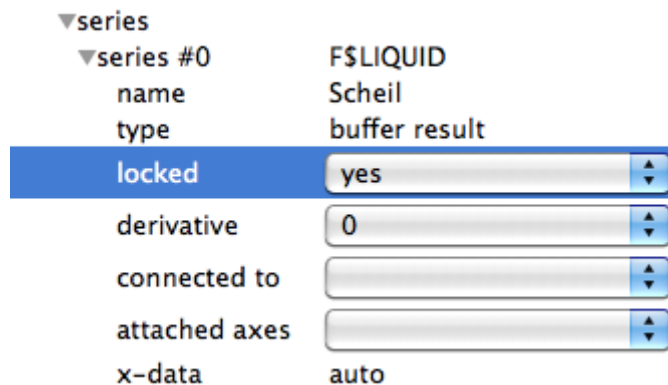
Then, we make sure that the just created buffer (**'Scheil with BD of C'**) is selected as current buffer in the options window and drag and drop the **'F$LIQUID'** variable into the plot (note that alternatively you can use the 'Lock and duplicate series' option accessible via the right

mouse button or the 'View' menu). Rename the new series to **'Scheil with BD of C'**. The new diagram looks like the following figure.
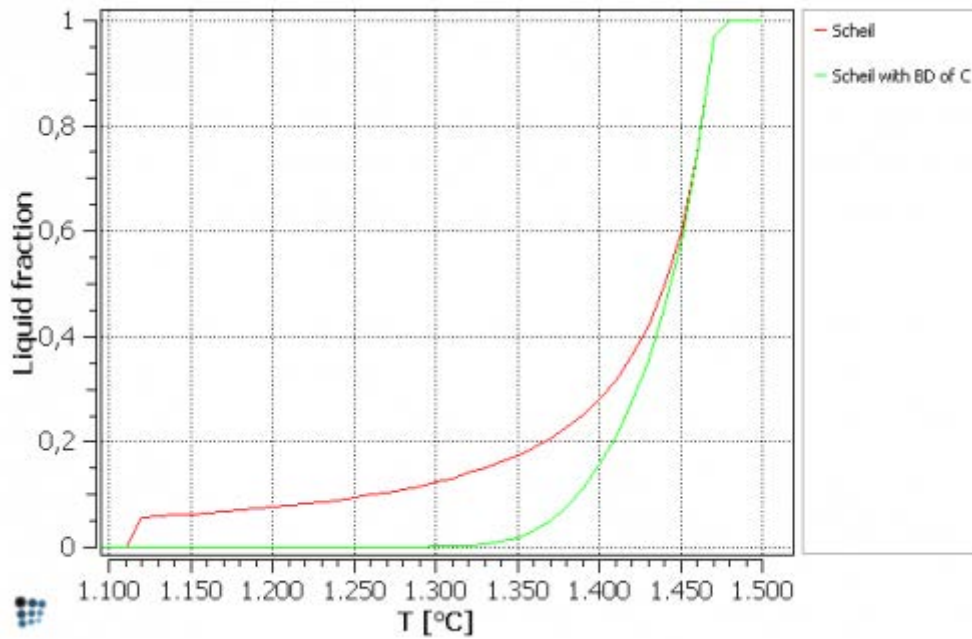
STEP 4: ADD THE EQUILIBRIUM SOLIDIFICATION PATH

Let us finally add the solidification temperatures for thermodynamic equilibrium conditions. To speed up the calculations, we **suspend all 'solid' phases which were needed for the Scheil calculations**. Open the **'Phase status'** dialog (**F8**). Set the **'suspended'** flag for each **'solid'** phase.
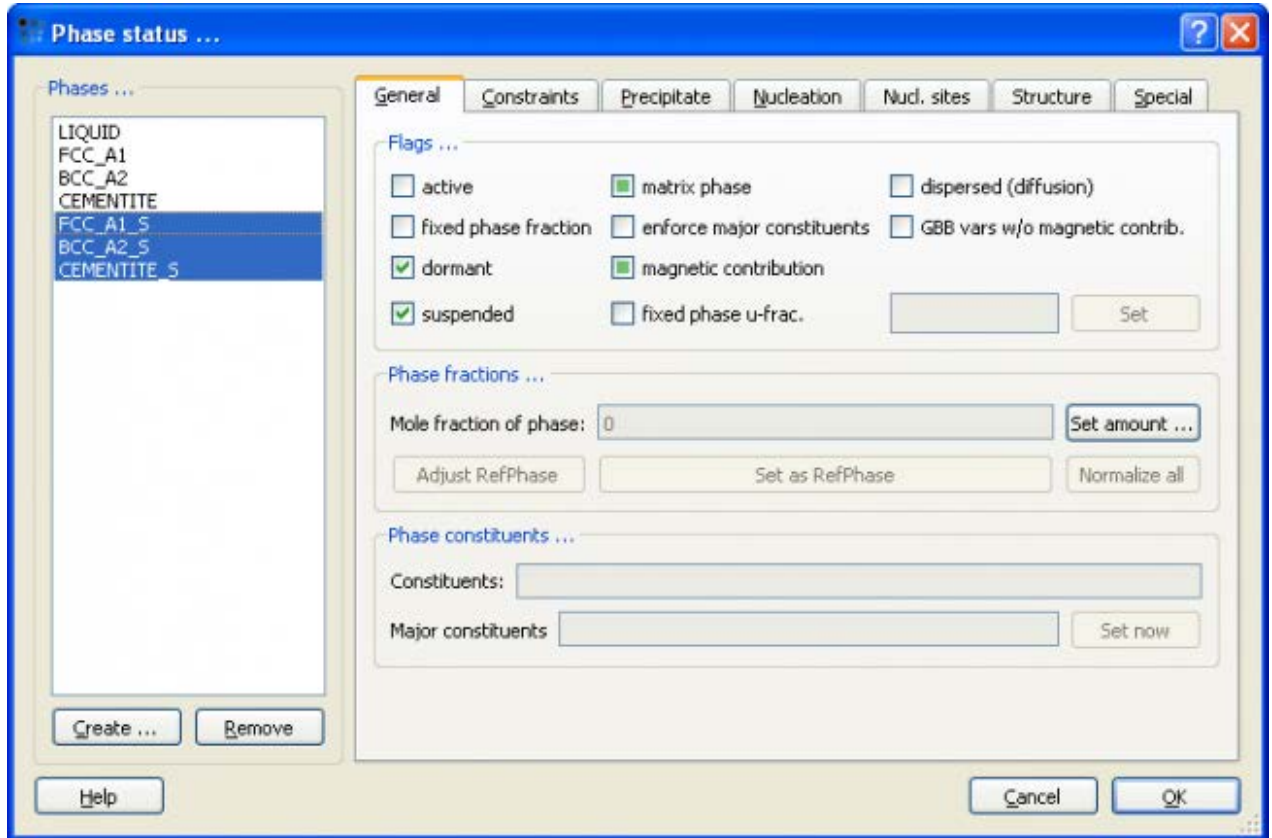
Create a new buffer with the name **'Equilibrium'**. Open the stepped calculation dialog (**Ctrl+T**). Calculate a stepped calculation with temperature as the variable between 1500°C and 1350°C in steps of 5. Press **'Go'** to start the calculation.
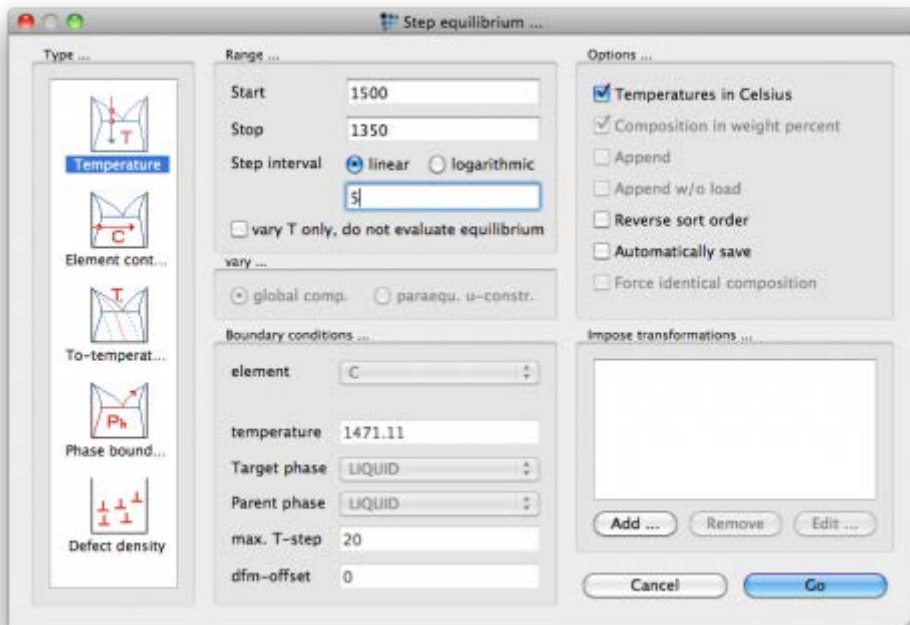
Change the buffer to be used in the diagram window to **'Equilibrium'** and drag and drop the **'F$LIQUID'** variable into the plot **after locking the previous series as done before**. Rename the current series and the diagram looks like this:
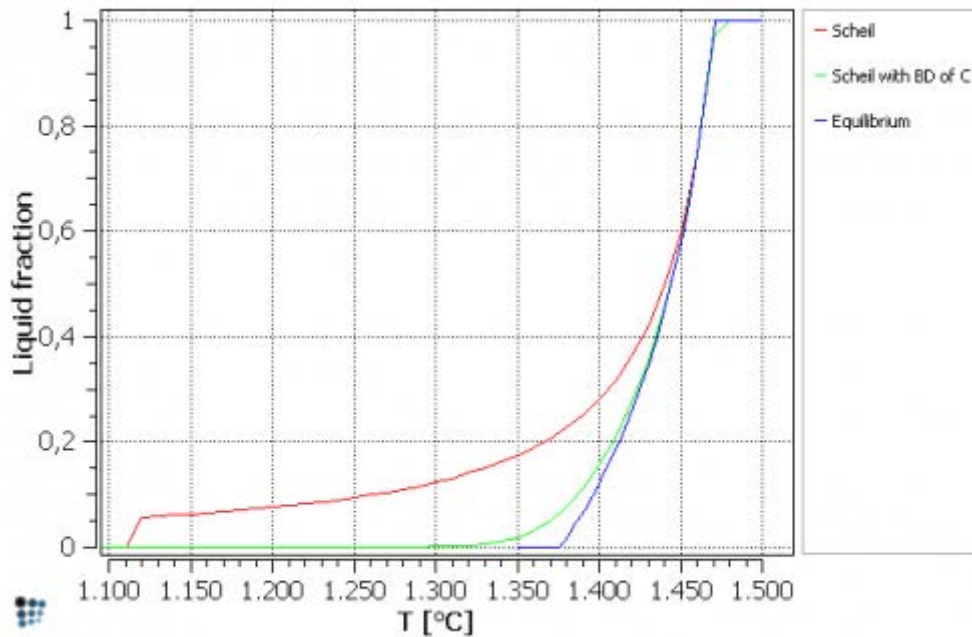
On changing the **'y-axis'** type to **'log'** and scaling from 0.01, the results finally display as
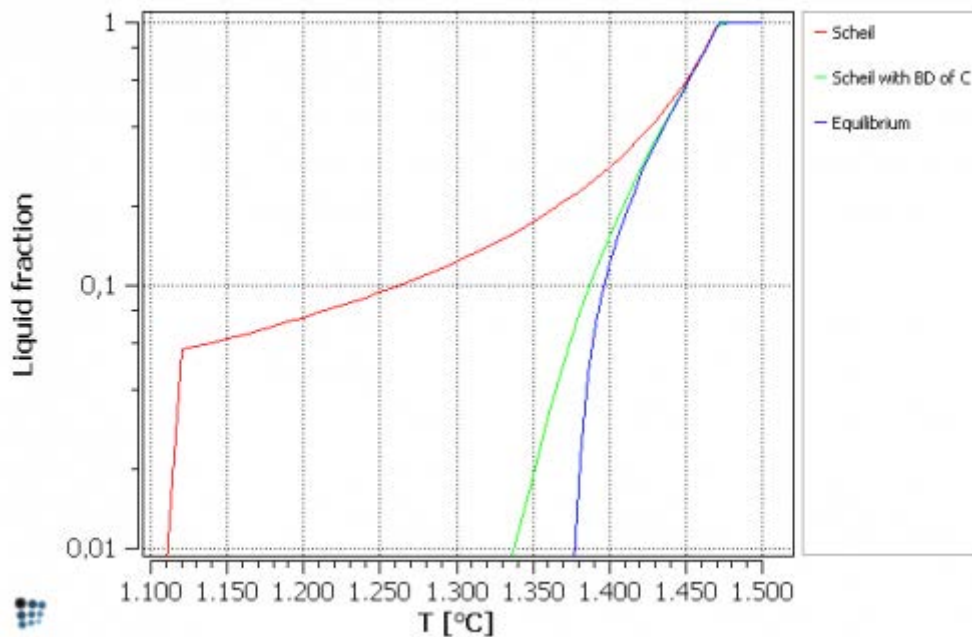
From this diagram, and with the assumption that all residual liquid freezes (solidifies) when 1% residual liquid is reached, the predicted solidification temperatures using the classical Scheil model, Scheil with back-diffusion and full thermodynamic equilibrium can be read as 1110, 1335 and 1380°C, respectively. Probably, 1335°C comes closest to the real, experimentally observed solidification temperature for this alloy composition.

CONSECUTIVE ARTICLES

The tutorial is continued in article T12 - Using the MatCalc console

[1)]**References**

[1] E. Kozeschnik, W. Rindler and B. Buchmayr, *„Scheil-Gulliver simulation with partial redistribution of fast diffusers and simultaneous solid-solid phase transformations"*, Int. J. Mater. Res., 98 (9), 2007, 826-831.

[2] W. Rindler, E. Kozeschnik and B. Buchmayr, *"Computer simulation of the brittle temperature range (BTR) for hot cracking in steels"*, Steel Res., 2000, 71 (11), 460-465.

[3] E. Kozeschnik, *"A Scheil-Gulliver Model with Back-Diffusion Applied to the Micro Segregation of Chromium in Fe-Cr-C Alloys"*, Met. Mater. Trans., 2000, 31A, 1682-1684.

T12: USING THE MATCALC CONSOLE

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb

CONTENTS:

- Getting help in the MatCalc console
- Obtaining lists of available commands for different modules
- Command syntax and abbreviations
- Example: calculating an equilibrium using the command-line
- Evaluating numerical expressions and variables
- Defining, using and plotting functions

BASICS

GETTING HELP AND LISTING AVAILABLE COMMANDS

Typing **'?'** or **'HELP_WORKSPACE'** in the **console window** shows a list of available commands.

```
_mcore: ?
--------------------------------------------------------------------------------
available commands in workspace module:
--------------------------------------------------------------------------------
?                          HELP_WORKSPACE            HELP_MODULE
ECHO                       !                         EXIT
USE_MODULE                 BACK_TO_MODULE            NEW_WORKSPACE
READ_WORKSPACE             SAVE_WORKSPACE            CLOSE_WORKSPACE
SET_WORKSPACE_PROPERTY     SET_WORKSPACE_INFO        LIST_WORKSPACE_INFO
RUN_SCRIPT_FILE            TEST_COMMAND              STOP_CURRENT_ACTION
STOP_RUN_SCRIPT            NEW_GUI_WINDOW            REMOVE_GUI_WINDOW
MOVE_GUI_WINDOW            SET_GUI_WINDOW_PROPERTY   UPDATE_GUI_WINDOWS
LIST_GUI_WINDOW_PROPS      LIST_ALL_GUI_WINDOWS      ALLOW_WINDOW_UPDATE
SET_PROGRESS_INDICATOR     CREATE_NEW_PLOT           SET_PLOT_OPTION
LIST_PLOT_OPTIONS          REMOVE_PLOT               LIST_ALL_PLOTS
COPY_PLOT_TO_CLIPBOARD     COPY_FRAME_TO_CLIPBOARD   EXPORT_PLOT_TO_FILE
EXPORT_FRAME_TO_FILE       LIST_CURRENT_DIRECTORIES  SET_APPLICATION_DIRECTORY
SET_WORKING_DIRECTORY
SHOW_EXPRESSION            SET_VARIABLE_VALUE
INPUT_VARIABLE_VALUE       REMOVE_VARIABLE           LIST_ALL_VARIABLES
LIST_INTERNAL_VARIABLES    SET_VARIABLE_STRING       INPUT_VARIABLE_STRING
FORMAT_VARIABLE_STRING     REMOVE_STRING_VARIABLE    LIST_ALL_STRING_VARIABLES
SEND_OUTPUT_STRING         SEND_CONSOLE_STRING       SEND_DIALOG_STRING
SET_FUNCTION_EXPRESSION    LIST_ALL_FUNCTIONS        REMOVE_FUNCTION
EDIT_SYMBOL                EDIT_PARAMETER            LIST_SYMBOLS
LIST_PARAMETERS
--------------------------------------------------------------------------------
use HELP_MODULE for module specific commands
--------------------------------------------------------------------------------
```

The commands listed above are part of the **'workspace'** module of MatCalc and relate to creating and modifying workspaces and windows within workspaces. As can be seen from the

last line of the above transcript, **'HELP_MODULE'** gives access to another series of commands relating to the current module of the program (**'core'**), i.e. the calculations themselves:

```
_mcore: help_module
-----------------------------------------------------------------------
available commands in mc_core module:
-----------------------------------------------------------------------
RESTART                       LICENSE_INFO            GIBBS_CALC_STATUS
LIST_DATABASE_CONTENTS        SELECT_ELEMENTS         SELECT_PHASES
SET_REFERENCE_ELEMENT         ENTER_COMPOSITION       SET_TEMPERATURE_CELSIUS
SET_TEMPERATURE_KELVIN        SET_PRESSURE            SET_AUTOMATIC_STARTVALUES
APPLY_TANGENT_CONSTRUCTION    CALCULATE_EQUILIBRIUM   SEARCH_PHASE_BOUNDARY
STEP_EQUILIBRIUM              LIST_EQUILIBRIUM        LIST_CORE_STATUS
SET_STEP_OPTION               LIST_STEP_OPTIONS       CHANGE_PHASE_STATUS
LIST_PHASE_STATUS             CREATE_NEW_PHASE        REMOVE_PHASE
<<CORE>>                      <<NODES>>               <<SYMBOLIC>>
<<IO>>                        <<PRECIPITATION>>       <<STATE>>
<<BUFFER>>                    <<TABLES/ARRAYS>>       <<TRANSFORMATIONS>>
<<HEAT_TREATMENTS>>           <<EXPORT>>
```

The **'mcore'** module contains several subsections, given in triangular brackets below the list of commands. These can be opened by typing in **'HELP_MODULE'** again with the name of the subsection. For example **'HELP_MODULE IO'** lists the input/output commands.

```
_mcore: help-module io
-----------------------------------------------------------------------
available commands in mc_core module: IO
-----------------------------------------------------------------------
OPEN_THERMODYN_DATABASE       TEST_EXIST_TD_DATABASE   READ_THERMODYN_DATABASE
READ_MOBILITY_DATABASE        TEST_EXIST_MOB_DATABASE  READ_PHYSICAL_DATABASE
TEST_EXIST_PH_DATABASE        SET_LOG_FILE             WRITE_BINARY_FILE
READ_BINARY_FILE              SET_AUTOSAVE_FILENAME    TEST_EXIST_FILE
```

NOTES ON SYNTAX

1. Although the commands listed above contain underscores **'_'**, the hyphen **'-'** can be used interchangeably with the underscore when typing **commands**. Note, however, that this is not the case in names of phases such as **'BCC_A2'**, which require the underscore.
2. Commands are case-insensitive.
3. Any unambiguous abbreviations of the commands are allowed. For example, **'open_th'** or even **'o_t'** are acceptable abbreviations of **'open_thermodyn_database'**. Using an ambiguous abbreviation, such as **'read'**, gives a list of all possible commands with that abbreviation, together with a message indicating that the command was ambiguous:

```
_mcore: read
READ_WORKSPACE
READ_THERMODYN_DATABASE
READ_MOBILITY_DATABASE
READ_PHYSICAL_DATABASE
READ_BINARY_FILE
*** error *** ambiguous command
_mcore:
```

EXAMPLE: CALCULATING AN EQUILIBRIUM USING THE COMMAND-LINE

The use of command-lines will be illustrated with a simple example: setting up a workspace and calculating an equilibrium at a single temperature. This is the same calculation as in Tutorial 2: an equilibrium at 700°C in a Fe-0.4 wt.% C system containing the phases LIQUID, FCC_A1, BCC_A2 and CEMENTITE.

Start with a new workspace. (Warning! Using the **'new_workspace'** command does not prompt the user to save any previously open workspace files, so make sure any necessary changes are saved first.)

```
_mcore: new_workspace
<script(0)>
<script(0)> $ running autonew.mcs script ...
<script(0)> m-gui-w 0 0 500 900 450
<script(0)> n-gui-w a6
<script(0)> m-gui-w . 500 0 500 450
<script(0)> n-gui-w a5
<script(0)> m-gui-w . 0 0 450 300
<script(0)> set-workspace-prop m n
<script(0)>
<script(0)> $ ready ...
<script(0)>
_mcore:
```

Open the thermodynamic database. This is equivalent to clicking **'Open'** in the **'Global > Databases'** dialogue box.

```
_mcore: open_thermodyn_database
name for thermodynamic database ('*' for list) /mc_sample_fe.tdb/:
```

The console prompts the user for the name of a database. The default option is given between slashes **'/../'** (By typing **'*'** and pressing **'enter'**, the content of the **…\MatCalc\database** directory is shown). Press **'enter'** to accept the default **'mc_sample_fe.tdb'** database. Find out which elements and phases are in the database using **'list_database_contents'**:

```
_mcore: list_database_contents
(e)quilib/(d)iffusion/(p)hysical /e/: e
equilibrium database file: C:/Programme/MatCalc/database/mc_sample_fe.tdb
# of elements in database: 15
    VA, AL, C, CR, CU, FE, MN, MO, N, NB, NI, SI, TI, V, W

# of phases in database: 15
LIQUID              FCC_A1              BCC_A2
HCP_A3              ALN                 CEMENTITE
CU_S                GRAPHITE            M23C6
M6C                 M7C3                LAVES_PHASE
KSI_CARBIDE         M3C2                SIGMA
V3C2                CR2VC2              FE4N
MN6N4               MN6N5               ZET
```

Select the required elements using **'select_elements c fe'**. A message appears to indicate that C has been selected, and Fe has been ignored because it was already selected by default.

```
_mcore: select_elements c fe
element 'C' selected
element 'FE' ignored
```

Next select the phases. Any unambiguous abbreviation is acceptable for the phase names. Messages appear to confirm that these phases have been selected.

```
_mcore: select_phases liq bcc fcc cem
phase 'LIQUID' selected
phase 'BCC_A2' selected
phase 'FCC_A1' selected
phase 'CEMENTITE' selected
```

Read in the thermodynamic data. This is equivalent to clicking **'read'** in the 'Databases' dialogue box.

```
_mcore: read_thermodyn_database
```

Enter the composition. There are three available unit qualifiers: x (mole fraction), u (u-fraction) and w (weight fraction). In addition, appending **'p'** to any of these gives the unit in percent. See the example below, in which the composition is specified in weight percent.

```
_mcore: enter_composition
unit qualifier (X/U/W + P) /x/: wp
enter amount (e.g. Mn=0.32 C=0.01): c=0.4
```

Open **'Databases'**, **'Composition'** and **'Phase Status'** from the **'Global'** menu and note that the system setup entered using the command-line is shown in the GUI windows. Console and GUI versions of commands can be used completely interchangeably. Set the temperature to 700°C. Note that there are two commands for temperature, **'set_temperature_celsius'** and **'set_temperature_kelvin'**, depending on the units of interest.

```
_mcore: set_temperature_celsius 700
```

Impose automatic start-values and calculate an equilibrium.

```
_mcore: set_automatic_startvalues
_mcore: calculate_equilibrium
```

Note the results in **'phase summary'** window: the stable phases are BCC_A2 and CEMENTITE as expected.

EVALUATING EXPRESSIONS

As well as entering commands, the console can be used to evaluate numerical expressions, MatCalc variables and user-defined expressions and functions.

NUMERICAL EXPRESSIONS

Any numerical expression can be evaluated using the command **'SHOW_EXPRESSION'** (**'show'** or **'sh'** are acceptable abbreviations):

```
_mcore: show 4/5
4/5 =
            0.8
_mcore: show pi
pi =
    3.14159265359
```

Note the priority rules and the use of parentheses to override these, e.g.:

```
_mcore: show 4/5*3
4/5*3 =
            2.4
_mcore: show 4/(5*3)
4/(5*3) =
    0.266666666667
_mcore: show 4+4*2
4+4*2 =
            12
_mcore: show (4+4)*2
(4+4)*2 =
            16
```

EXPRESSIONS IN X

Expressions in terms of the current value of the stepped variable, x, can be evaluated using **'show_expression'**, as shown below. (The value of x is currently zero because no stepped calculation has so far been performed in this workspace.)

```
_mcore: show 3*x
3*x =
                            0
```

Functions in x can be defined and then evaluated.

```
_mcore: set-function-expression
which function: function1
enter expression: 3*x
_mcore: show function1
function1 =
             0
```

Pressing the up-arrow recalls the latest command to be entered. Further use of this up-arrow scrolls through the command history in reverse chronological order. Commands are given with the full names and chosen options, e.g.:

```
_mcore: SET_FUNCTION_EXPRESSION function1 3*x
```

The command-line can then be edited, e.g. replace **'function1'** by **'function2'**:

```
_mcore: SET_FUNCTION_EXPRESSION function2
enter expression: x**2
```

This is the expression for x^2. The syntax **'x^2'** can also be used for the same purpose:

```
_mcore: SET_FUNCTION_EXPRESSION
which function /function2/: function3
enter expression: x^2
```

The functions just defined can now be found by opening the **'Functions'** tab in **'Global > Variables & functions'**, and in the **'variables'** window under **'functions'**. They can be plotted in a new window as follows:

Firstly, create a new window and enter the window-type code. These codes can be found under **'View > Create new window'**. The standard x-y plot is **'p1'**.

```
_mcore: new_gui_window
enter window-type code: p1
```

Next, add a new series using set-plot-option and choosing the following options (press Enter, if there is no sign behind the colon):

```
_mcore: set-plot-option
enter plot ID /1/:
(t)itle/(a)xis/(l)egend/(g)rid/(h)istogram/tt(p)/(s)eries: s
(n)ew/(e)dit/(r)emove/rena(m)e/(l)ock/(d)uplicate and lock
deri(v)e/(c)onvert to table: n
(b)uffer results/(t)able/experimental data/(f)unction/expression: f
expression in variable 'x': function1
definition range /auto/: -10..10
```

Finally, add the other two series by recalling and editing the previously used command.

```
_mcore: SET_PLOT_OPTION 1 S N F function2 -10..10
_mcore: SET_PLOT_OPTION 1 S N F function3 -10..10
```

The resulting plot should look like this:
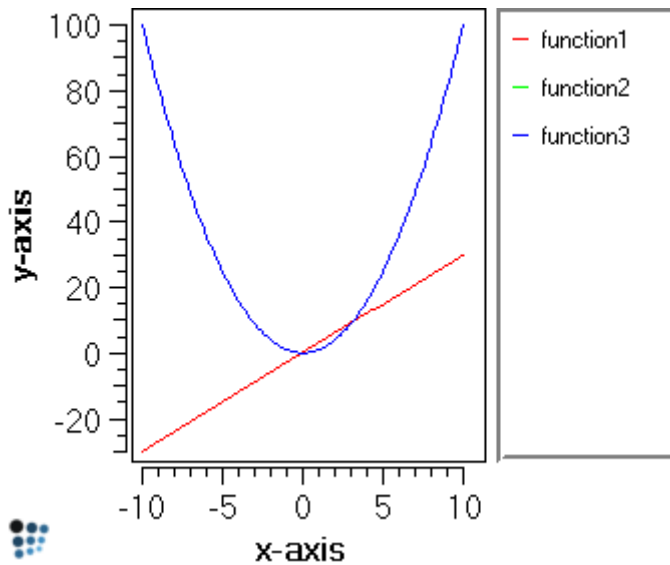
EXPRESSIONS USING MATCALC VARIABLES

It is also possible to define functions made up of MatCalc variables. Here, two functions similar to those discussed in Tutorial 6 are defined. The built-in variables can be copied and pasted from the **'variables'** window to the console using the right-click menus or Ctrl+C and Ctrl+V.

```
_mcore: SET_FUNCTION_EXPRESSION function4 F$BCC_A2*X$BCC_A2$C
_mcore: SET_FUNCTION_EXPRESSION function5 F$CEMENTITE*X$CEMENTITE$C
```

These new functions can then be evaluated using **'show'**:

```
_mcore: show function4
function4 =
   0.000627080528289
_mcore: sh function5
function5 =
   0.0177039299864
```

Expressions can be built up from existing functions and variables:

```
_mcore: show function4+function5
function4+function5 =
   0.0183310105147
```

Below, it is confirmed that, at 700°C, function4 + function5 = XS$C i.e. all the carbon in the system is in the form of either BCC_A2 or cementite, since these are the only two phases to be stable at this temperature.

```
_mcore: show XS$C-(function4+function5)
xs$C-(function4+function5) =
            0
```

The next tutorial discusses the use of command-lines in scripts to facilitate repetitive or complex tasks.

CONSECUTIVE ARTICLES

The tutorial is continued in article T13 - Introduction to scripting (1: Equilibrium calculations)

T13: Introduction to scripting (1: Equilibrium calculations)

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb

Contents:

- Purpose of scripts
- Writing a script to perform a stepped calculation and display the results

Introduction

Utility of scripts

A script is a text file, containing a list of commands to be executed in order from top to bottom. They are particularly useful to speed up routine or repetitive operations. Once a script file has been created, it can easily be modified to serve a new purpose, for example by changing the elements or phases in the system. Script files, consisting only of text, are also much smaller in size than MatCalc workspace files, especially those resulting from precipitation calculations.

Individual scripts can also be grouped into master-scripts; this facilitates, for example, calculations involving multi-stage heat treatments. Some sample scripts are provided with MatCalc. You will find them in the subdirectories of
'MatCalc/scripts/script_menu/templates'. Of course, you can also edit them in MatCalc by clicking on **'Open template…'** in **'Script'** menu.

Writing a script

There are two ways of creating a script:

1. In MatCalc, choose **'New'** from the **'File'** menu and select **'Script file'** from the drop-box. Note that it is possible to have any number of script files open simultaneously with a MatCalc workspace file. **'Save'** or **'Save as'** will save the script file if its window is highlighted, otherwise the workspace will be saved. Recently used script files can be found in a list under **'File > Recent files'**.
2. Alternatively, create the new script in any text editor (which saves files as plain text), such as notepad, emacs, vi or any of the many text editors available in different Linux distributions.

N.B.- The MatCalc scripts have '.mcs' extension so it is important to set (or change) the extension of the created file!

Editing a script

There are also two ways of editing an existing script:

1. In MatCalc, using **'File > Open'** or clicking on 📁 icon in the toolbar (keyboard shortcut **'Ctrl + O'**). Select the filter to **'MatCalc script (*.mcs)'** files
2. Alternatively, you can use any text editor (which saves files as plain text).

EXECUTING A SCRIPT

And again, there are two ways of executing a script in MatCalc:

1. Using **'Extra > Run script'** or clicking on 🔳 icon in the toolbar (keyboard shortcut **'Shift + F2'**)
2. Double-clicking on the **'.mcs'** file icon

EXAMPLE: A STEPPED EQUILIBRIUM

This example will show how to write a script to perform the stepped calculation in Tutorial 3 and display the results.

COMMENTS

It is always advisable to comment the script extensively so as to help other users (or oneself several months later!) to understand the aim of the calculation, assumptions, etc. Any line prefixed with a **'$'**-sign will not be interpreted as a command. The **'$'**-sign can also be inserted part-way through a line; the rest of the line will be treated as a comment.

```
$ This whole line is a comment.
NEW_WORKSPACE $ The rest of this line is a comment.
```

Both comments and commands are shown line-by-line in the console when the script is executed, but prefixing a comment or a command with the **'@'**-sign hides the line so that it does not appear in the console output.

At the beginning of the script, enter some preliminary comments, containing such information as: the name of the file, the current version of MatCalc (available from Help > About), the current version of the scripting language and a brief summary of the purpose of the script.

```
$ Script T13
$ This is a script for MatCalc version 5.41
$ MatCalc script version 1
$ Calculating equilibrium phase stability in Fe-0.4C wt.%
```

Save the file as **'T13.mcs'**

CALCULATING AN EQUILIBRIUM

The first executable line in the script creates a new workspace (**N.B.- Any previously open workspace will be closed without warning.**)

```
@$********************************
$ Create a new workspace file
@$********************************
new_workspace $this executes 'autonew.mcs' script
```

The next lines are to enter some workspace information to describe the ideas, assumptions etc. used in the calculation. This information can be found in **'File > Workspace info'**. The **'+'**-sign continues the text on a new line.

```
@$********************************
$ enter workspace info
@$********************************
@ set-workspace-info Script T13
@ set-workspace-info +Calculation of equilibrium phase stability
@ set-workspace-info +in Fe-0.4C wt.% system
@ set-workspace-info +with phases LIQUID, BCC_A2, FCC_A1 and CEMENTITE.
```

Next, add the command-line to open the thermodynamic database.

```
@$********************************
$ open the thermodynamic database
@$********************************
open_thermodyn_database
```

If the line is put in as above, the script will stop at this point and prompt the user for the name of a thermodynamic database. The output in the console window is as follows:

```
<script(0)> $ open the thermodynamic database
< script(0)> open_thermodyn_database
name for thermodynamic database /mc_sample_fe/:
```

(Press **'enter'** to select the default option.) Leaving out the arguments of the command in this way allows for interactivity in scripts. If, instead, the script is intended to be fully automatic, the argument should be put after the command on the same line. Replace the above line with the following:

```
open_thermodyn_database mc_sample_fe.tdb
```

The next parts of the script are to set up the system, set the temperature and calculate an equilibrium. These commands have already been seen in Tutorial 12.

```
@$********************************
$ select elements and phases
@$********************************
select_elements c fe
select_phases liq bcc fcc cem
@$********************************
$ read in the thermodynamic data
@$********************************
read_thermodyn_database
@$********************************
$ enter the composition
@$********************************
enter_composition wp c=0.4
```

```
@$*********************************
$ set the temperature and calculate an equilibrium
@$*********************************
set_temperature_celsius 700
set_automatic_startvalues
calculate_equilibrium
```

STEPPED CALCULATION

In the line below, the argument **'r'** means range, and the numerical values are the start, end and step interval.

```
@$*********************************
$ define step parameters and make stepped calculation
@$*********************************
set_step_option r 400 1600 L 25
step-equilibrium
```

GRAPHICAL OUTPUT

The final part of the script is concerned with graphical presentation of results. The following line creates a new GUI window to contain the plot. As was seen in Tutorial 12, the code **'p1'** is used to open an XY-plot.

```
@$*********************************
$ graphical output
@$*********************************
new-gui-window p1
```

The following three lines change the default x-data from **'StepValue'** to temperature in Celsius, set a default x-axis to be used for all plots, and provide a title for this axis. The **'.'** in these lines refers to the ID of the last-used window, which in this case is the p1 window which has just been created.

```
set-gui-window-property . x t$c
set_gui_window_property . s u y $ set default x-axis to be used for all
plots
set_gui_window_property . s t Temperature [°C] $ title for default x-axis
```

The line below adds a title to the diagram. This first diagram is to be a plot of phase fraction versus temperature.

```
set-plot-option . t Phase stability in Fe-0.4 wt.% C
```

The following lines label the y-axis, change the 'factor' of the y-axis from 1 to 100 to display the calculated phase fraction directly in percent, set the axis type to logarithmic and modify the axis scaling.

```
set-plot-option . a y 1 t Phase fraction [%]
set-plot-option . a y 1 f 100
set-plot-option . a y 1 y log $ changes axis type to log
set-plot-option . a y 1 s 1..100 $ modifies axis scaling
```

The first series is inserted using **'set-plot-option . s n b f$liquid'**; this is the phase fraction of liquid. The name of the series, as it will appear on the legend, is then edited using **'set-plot-option . s m -1 f$liquid Liquid'**. This changes the name from its automatic value (f$liquid) to **'Liquid'**.

```
set-plot-option . s n b f$liquid
set-plot-option . s m -1 f$liquid Liquid
```

These commands are repeated for the other phases. Note the use of the HTML markup tags to give the subscript in **'Fe₃C'**.

```
set-plot-option . s n b f$bcc_a2
set-plot-option . s m -1 f$bcc_a2 Ferrite
set-plot-option . s n b f$fcc_a1
set-plot-option . s m -1 f$fcc_a1 Austenite
set-plot-option . s n b f$cementite
set-plot-option . s m -1 f$cementite Fe₃C
```

The three lines below move and resize the window, update its contents and set the style-sheet to coloured with no symbols. In the first of these lines, the first two numbers define the position of the window, the second two define the width and height.

```
move_gui_window . 20 20 800 1000
update-gui-window .
set_gui_window_property . y col_no_symb $sets style-sheet to colour with no
symbols.
```

Another plot can be added in the current window as shown below

```
create_new_plot x .
```

The newly created plot now becomes the **'current'** plot and can be referred to as **'.'** when it is being modified with set_plot_option:

```
set_plot_option . t Composition of phases
set-plot-option . a y 1 t Carbon content [wt.%] $ label on y-axis
set-plot-option . s n b x$liquid$C $wp $ adding the first series…
set-plot-option . s m -1 x$liquid$C Liquid $… and changing its name.
set-plot-option . s n b x$bcc_a2$C $wp
set-plot-option . s m -1 x$bcc_a2$C Ferrite
set-plot-option . s n b x$fcc_a1$C $wp
set-plot-option . s m -1 x$fcc_a1$C Austenite
set-plot-option . s n b x$cementite$C $wp
set-plot-option . s m -1 x$cementite$C Fe₃C
```

The script can be concluded with the following line, which should appear in the console when the script has been executed without any errors.

```
$ *** DONE ***
```

The final diagrams should look like this:
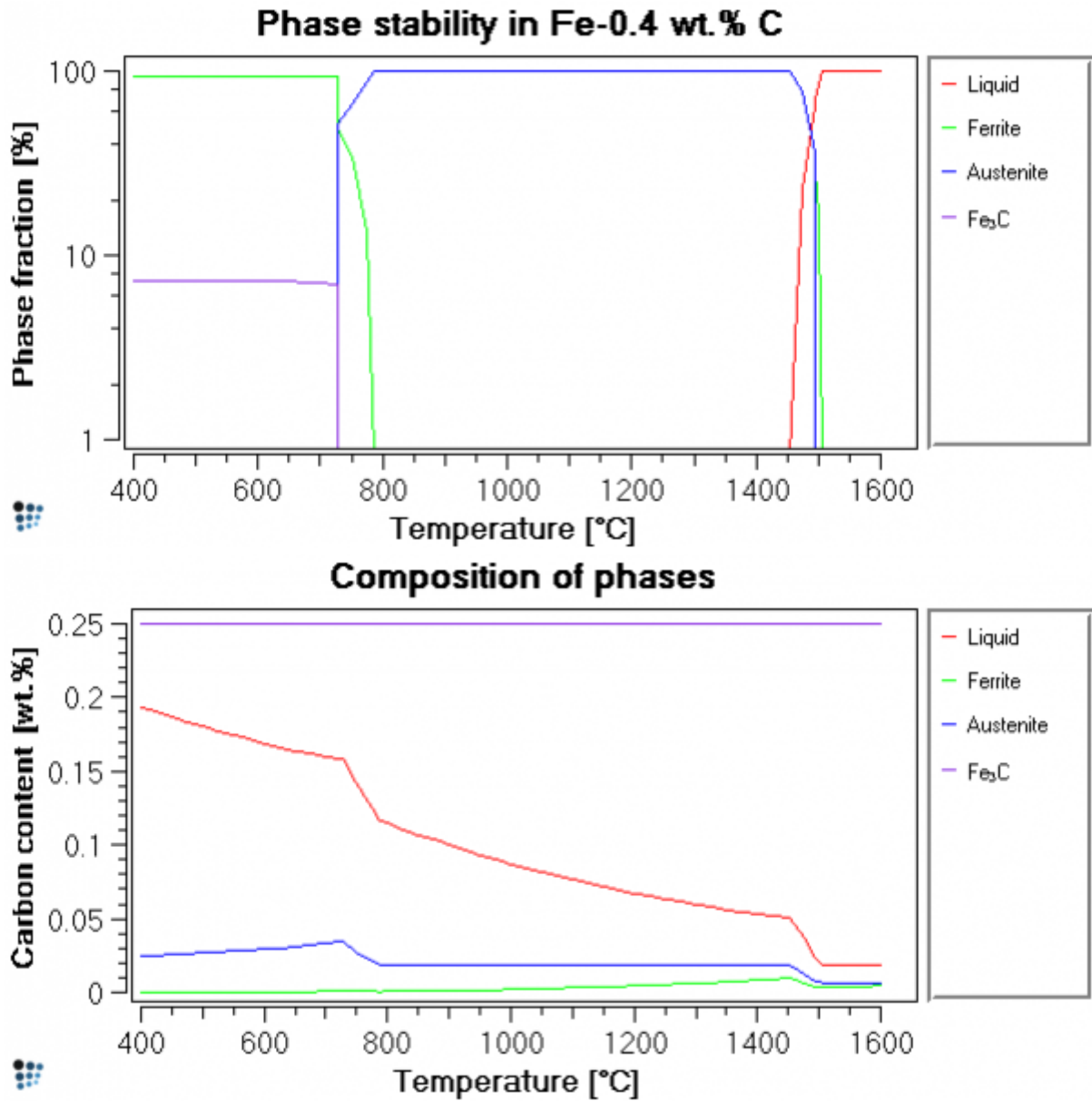
CONSECUTIVE ARTICLES

The tutorial is continued in article T14 - Introduction to precipitation calculations

T14: INTRODUCTION TO PRECIPITATION CALCULATIONS

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb; mc_sample_fe.ddb

CONTENTS:

- Precipitation of cementite in a ferritic matrix in Fe-0.2 wt.% C
- Creating a precipitation domain
- Creating a precipitate phase
- Mobility and physical data
- Plotting and interpreting calculation results

SETTING UP THE SYSTEM

A. THERMODYNAMIC SETUP

The first step is to set up the thermodynamics of the system. In the new workspace, open **'Global > Databases'** and select the elements Fe and C. For a precipitation calculation, it is only necessary to include the phases which are directly involved in the precipitation, i.e. the precipitating phase and the matrix in which it forms. This example considers the precipitation of cementite in ferrite, so the two phases to be selected are BCC_A2 and CEMENTITE. When the thermodynamic data have been read in, open **'Global > Composition'** and enter the carbon content of 0.2 wt.%.

B. PRECIPITATION DOMAIN

The next two steps are to define and configure the precipitating phase and the domain in which it will form. These two steps can be done in either order, but in this example, the precipitation domain will be set up first.
Open **'Global > Precipitation domains'** and click on the **'New'** button towards the bottom left. A box will appear, prompting for a name for the new domain. Any name can be chosen here, for example **'Ferrite'** or **'Matrix'** and click **'OK'**.
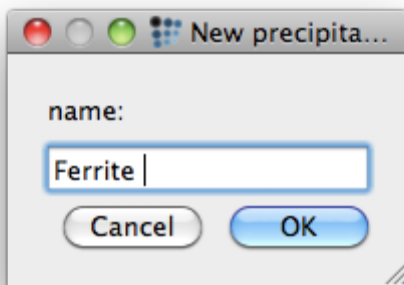
On the **'Phases'** tab, choose **'BCC_A2'** from the drop-box to associate this phase with the newly defined domain. Leave the rest of the settings as they are, and click **'OK'**.
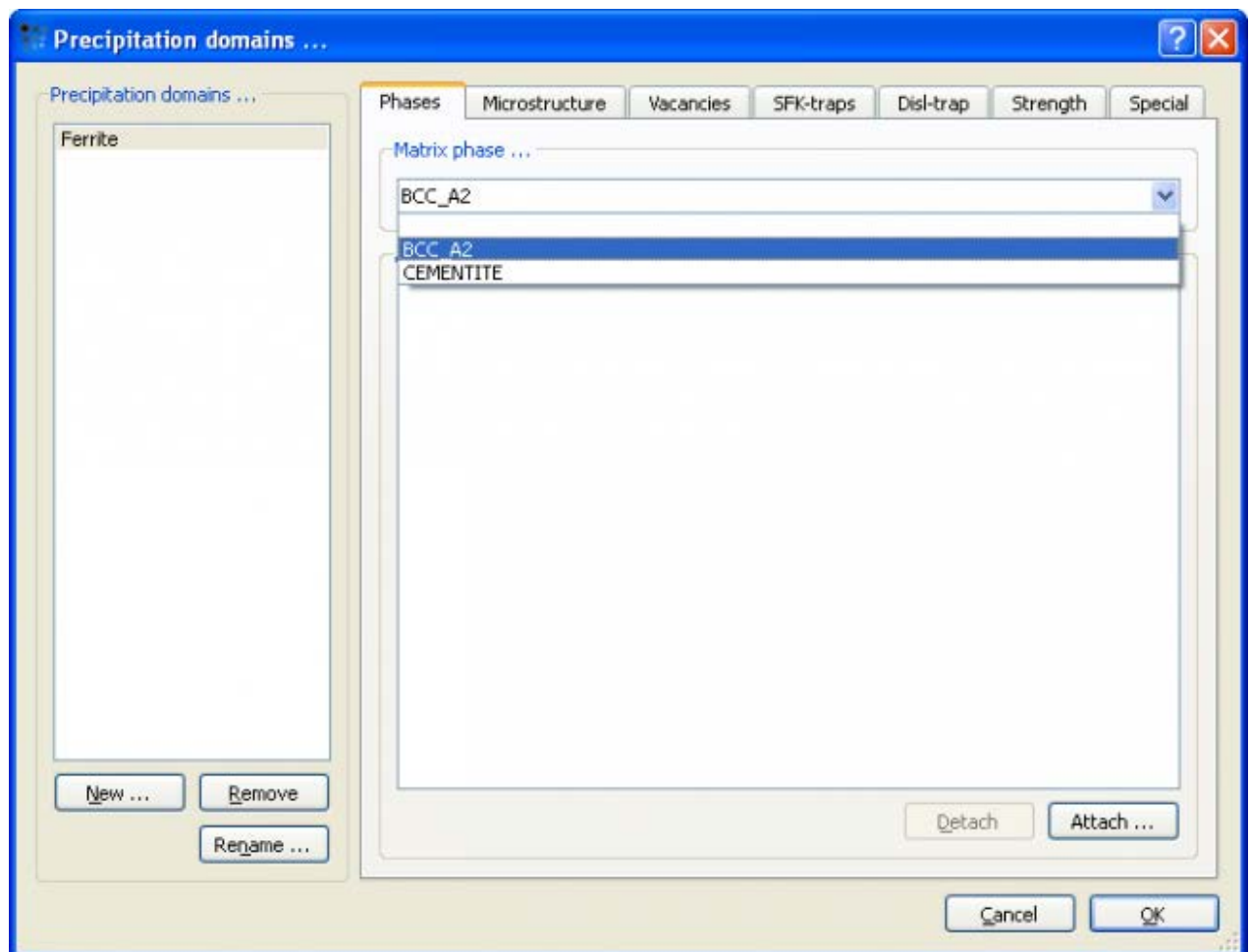
C. Precipitate phase

To create the precipitate phase, open **'Global > Phase status'**. In the **'Phases'** list on the left-hand side, select **'CEMENTITE'** and click on **'Create'**. Select **'precipitate (_Pnn)'** from the drop box which opens.
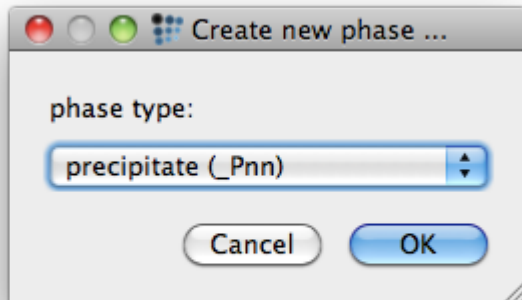
A new phase, CEMENTITE_P0 appears in the phase list; click on this to select it. Open the **'precipitate'** tab, and enter **'250'** in the **'# size classes'** box, click on **'Initialize'** and accept the warning message. The precipitates are considered as belonging to a number of classes of particles with the same radius and composition. Classes are created, rearranged and deleted during the calculation, allowing simulation of the precipitate size distribution. The choice of the number of classes represents a trade-off between calculation time and required precision. If only average properties, such as the mean precipitate radius, are of interest, then it is sufficient to use a small number of classes such as 10 or 20. By contrast, to obtain the best possible simulation of size distribution, the number of classes should be increased to a higher value, such as 250 as used here. Leave all the other settings in this tab as they are. In the **'Attached to pd'** drop box select the created domain (**'Ferrite'**)
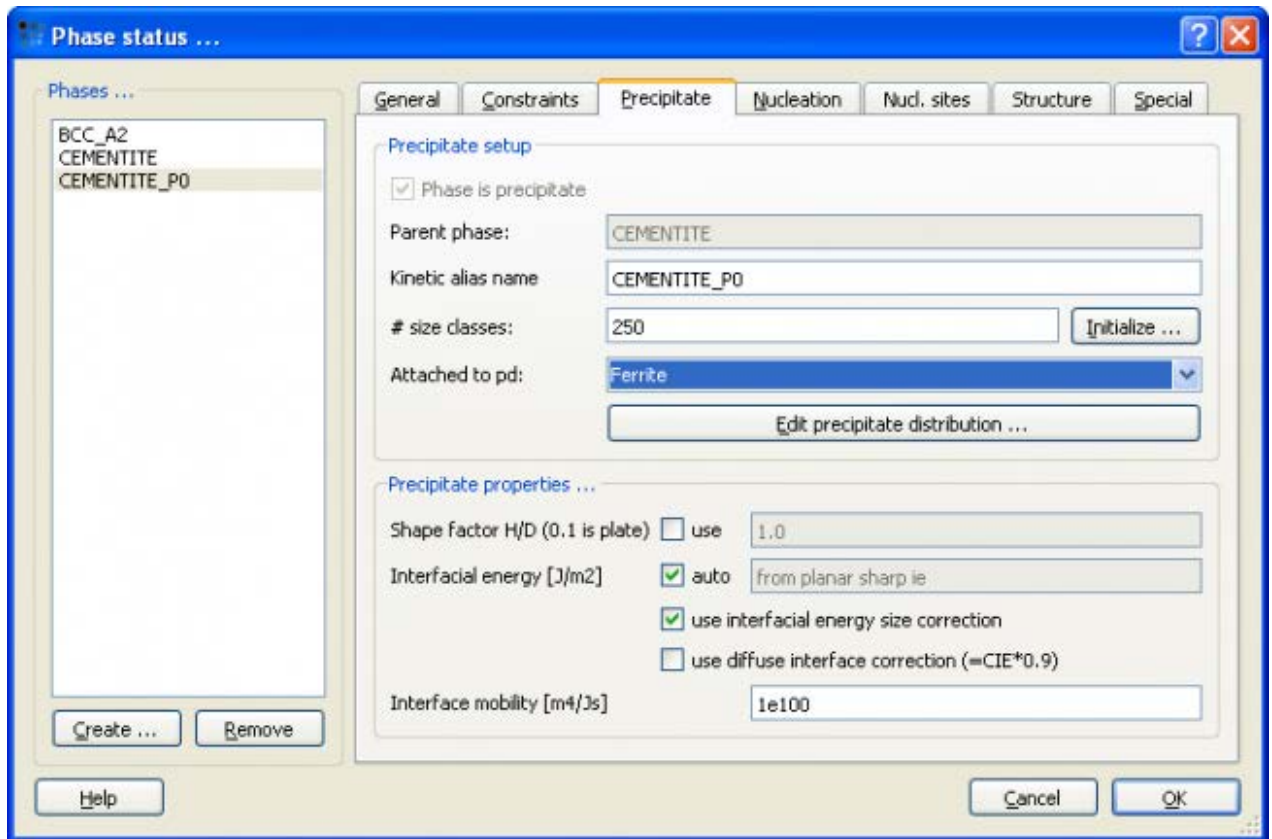
Open the **'nucleation'** tab. If the contents of the **'Nucleation model'** and other drop-boxes are not visible, click on another phase in the phase list at the left-hand side, then back on **'CEMENTITE_P0'**, and this will load the text.

In the **'Nucleation sites'** part of this tab, remove the tick-mark by **'bulk (homogeneous)'** and instead click in the box beside **'dislocations'** . Click on **'OK'** to save these settings and return to the main screen.
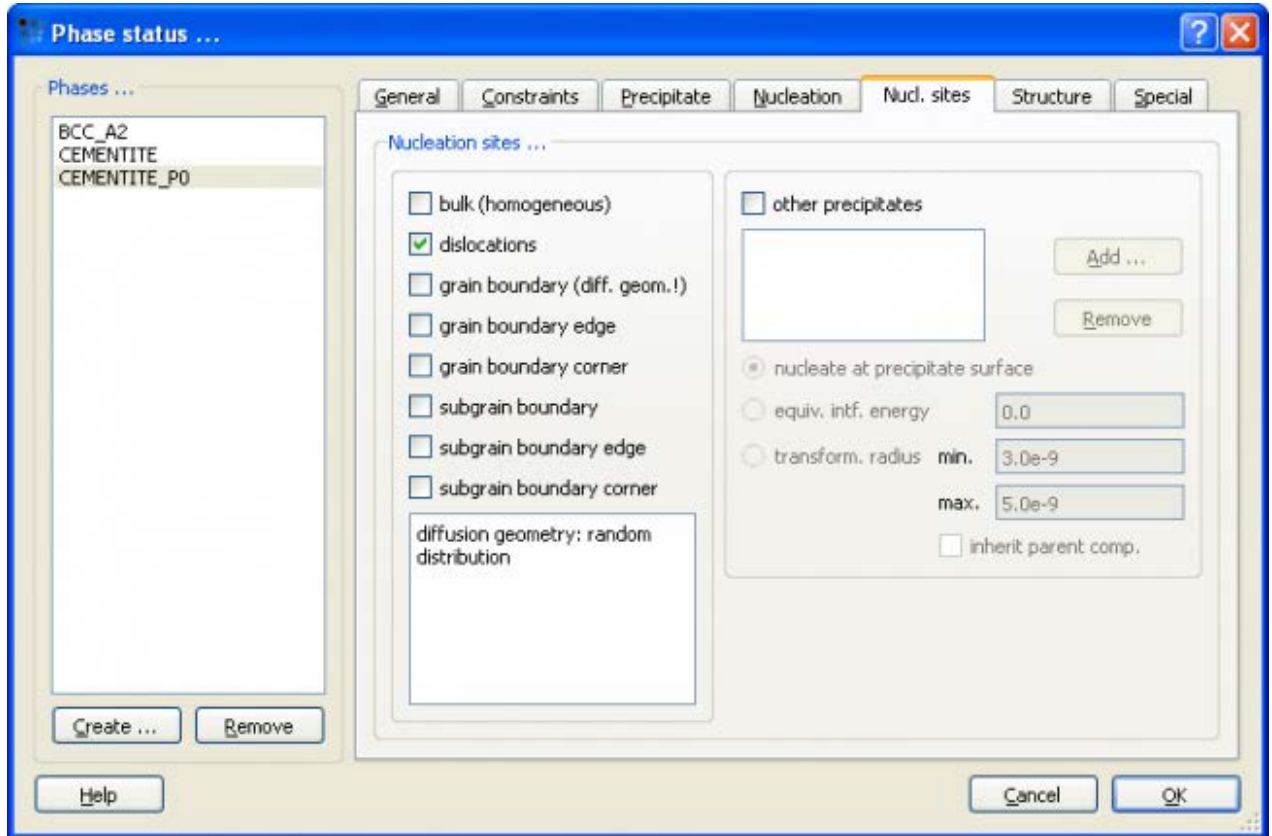
D. LOADING MOBILITY DATA

Simulations of precipitation require not only thermodynamic data (already loaded in step A) but also mobility data, from which the diffusivities of the elements in the phases can be calculated. Read in the mobility data by opening **'Global > Databases'** and select **'Diffusion data'** on the left side. Click on **'Read'** and open **'mc_sample_fe.ddb'** database. Click on **'Close'**
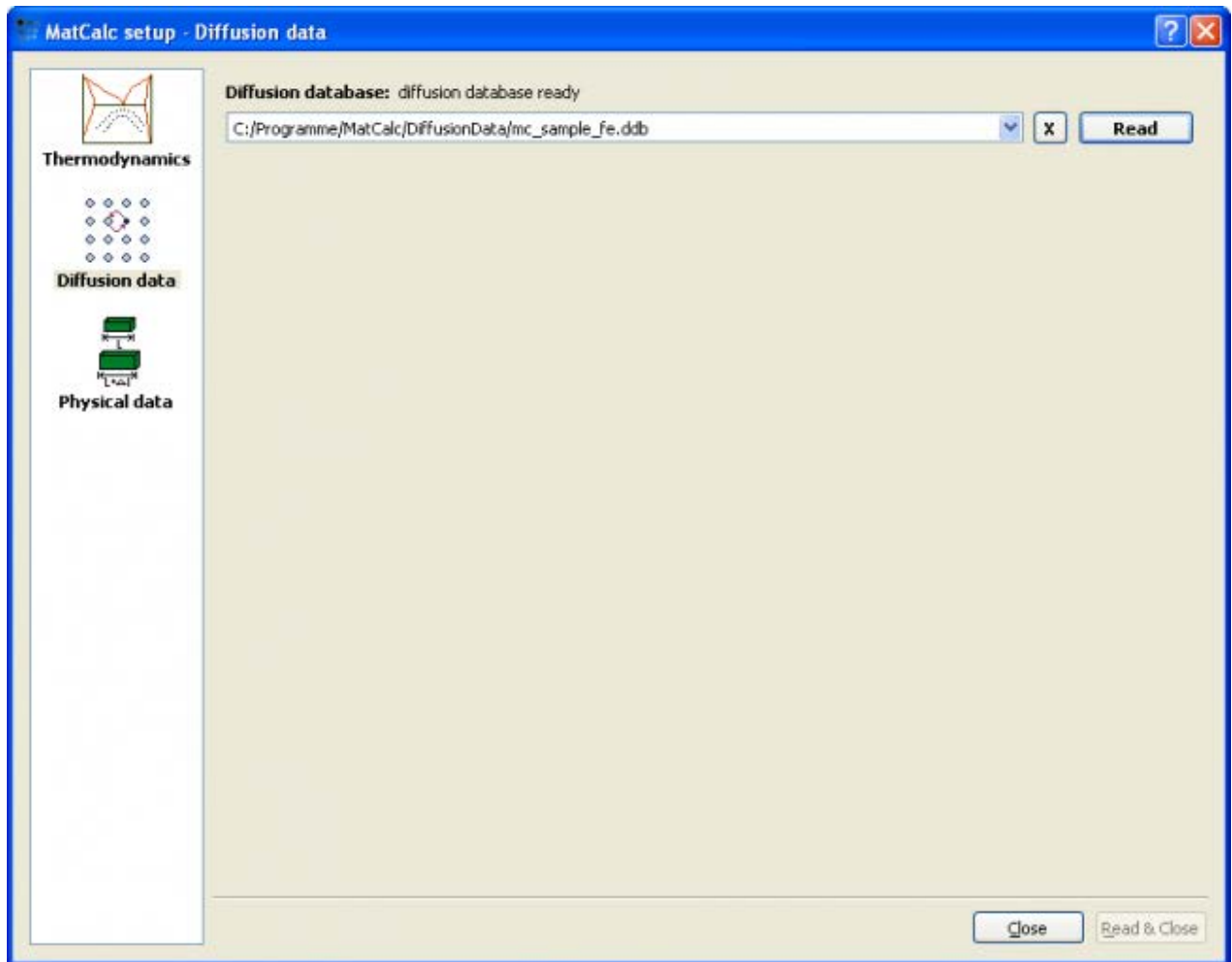
E. CREATING PLOTS FOR THE OUTPUT

Create a new **'Plot: XY-data'** window. Drag and drop **'F$CEMENTITE_P0'** from the variables window to this plot. In the **'options'** window, set **'default x-axis'** to **'log'** type and select **'yes'** for **'use for all plots'**. Change the title of **'default x-axis'** to **'time [h]'** and the factor to **'1/3600'** to convert seconds into hours. The title of the **'plot #0'** should also be changed to **'Phase fraction of cementite precipitates'** and the title of y-axis to **'Phase fraction'**. Next, create a new window **'Plot: precipitate distribution - histogram'** (p5) window. Select **'CEMENTITE_P0'** from the box which opens and click **'OK'**. In the **'options'** window, change the number of **'# size classes'** for this histogram to **'20'**. Set the x-axis label to **'Precipitate radius [nm]'**. In the **'factor'** line for this x-axis, enter **'1e9'**. This expresses the particle radii in nanometres instead of metres, making the scale easier to read. Change the y-axis label to **'Number of precipitates'**.
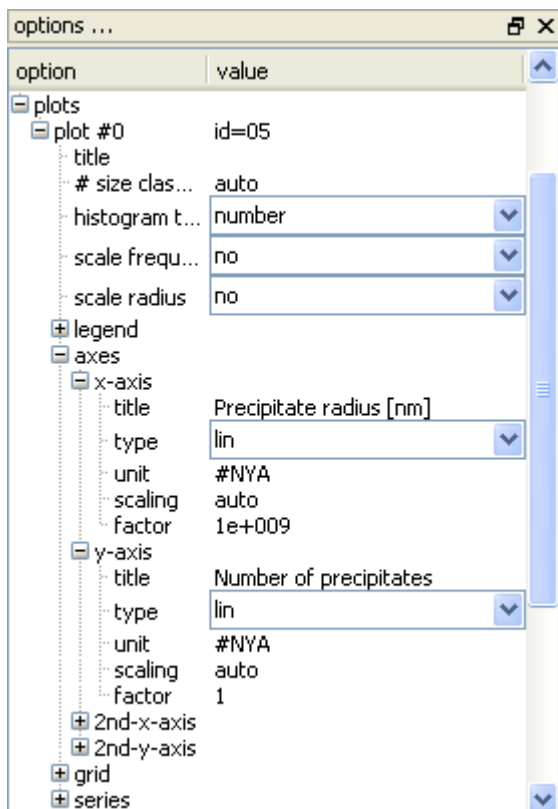
Both the histogram and the plot of phase fraction against time are updated during the calculation, so it is possible to follow the evolution of the size distribution and the phase fraction as the calculation takes place.

THE CALCULATION

As the introduced number of classes is quite large (as defined in p. 1.D.), it will be beneficial to modify the algorithm used for the calculation. To do this the numerical limits describing the increase of the nucleation density in the **'convergence control'** field should be changed. Up to now, this can be only modified via console commands. Type the following command-line in the console:

```
set-simulation-parameter c n b 1,05
```

Calculate an equilibrium at 600°C in the usual way. Open **'Calc > Precipitate kinetics'** or click on the icon (keyboard shortcut: **'Ctrl + K'**). Enter **'3.6e5'** as the simulation end time. This is in seconds, so is equivalent to 100 hours. Note that in the 'Temperature control' section, an isothermal heat-treatment at 600°C has been selected by default; leave this setting as it is.

To give more frequent updates of the graphs on the screen, the **'Update output every'** number can be decreased from 100 to 50. However, this will slow down the calculation somewhat, so it is probably not advisable on slow machines. Leave the other settings as they are, and click on **'Go'**.
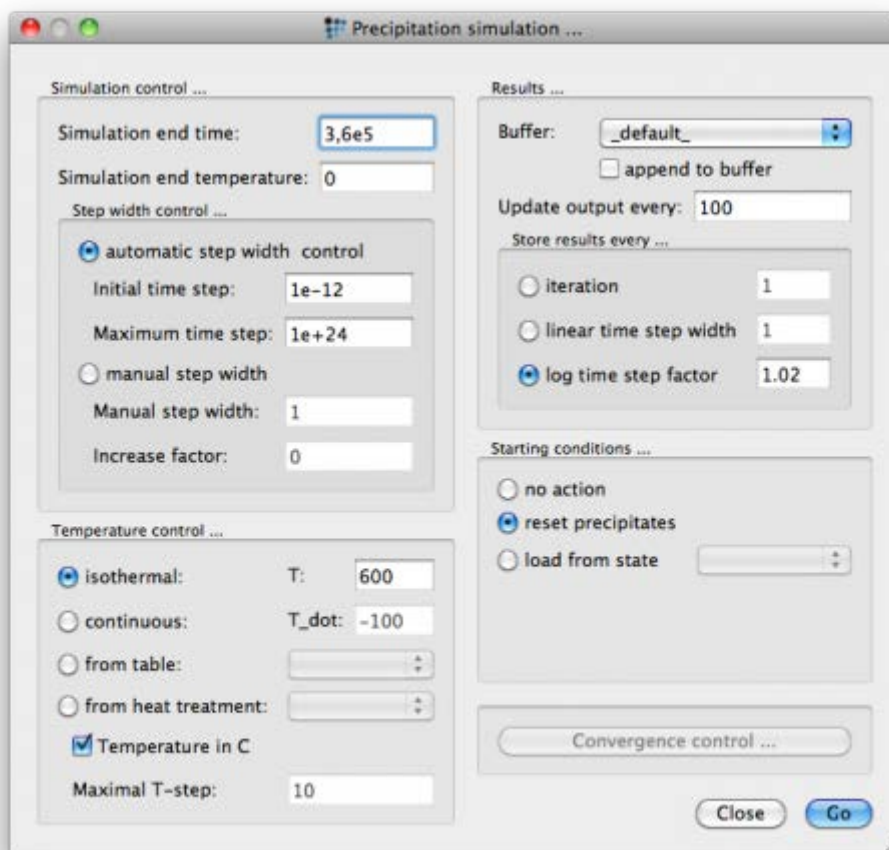
The information in the **'Output'** window gives a summary of the current system composition, simulation time

```
******** isothermal,T=873.16 K (600 C)
************************************************************
1, recs=1; its=1/1, dt=1e-012, time: 1e-012s (2.778e-016h), T=600 C (873.2
K), on Tue, 16:40:26
#Ferrite: BCC_A2, sv=6.13e-010 (sve=6.13e-010), dcf=1 (dt=0, -)
FE +9.90768e-001(+0.00e+000) C +9.23192e-003(+0.00e+000)
——————————————————————————————————-
CEMENTITE_P0: nucl-site: d, nucl-dfm=6840.7, ans=4e+021
+ CEMENTITE_P0 precipitation started at 1.9531e-008 s, T=600 °C (873.16 K)
```

- First line:

1 -Number of iterations.

recs -Number of records in buffer.

dt -Last time step.

time -Absolute simulation time in [s].

T - Current temperature in [°C] (in [K]).

- Second line:

#Ferrite - Precipitation domain, BCC_A2 - matrix phase,

sv - current vacancy concentration

sve - equilibrium vacancy concentration

dcf - diffusion correction factor due to the presence of the excess vacancies

damping feature (**dt=0,-**) - maximum time step allowed due to the matrix condition

- Third line:

FE +9.95367e-001(+0.00e+000) - Composition of matrix

- Fourth line:

CEMENTITE_P0: - Precipitate phase

(0/…./0e+000) - (number of classes used / '+', '-' or '.', meaning: New class built, class deleted or no change / Number of precipitates for this phase)

f - mole fraction of precipitate phase

rm - mean radius of precipitate phase

dfm - driving force for formation of phase in [J/mol]

nucl-dfm - driving force for nucleation in [J/mol]

ans - available nucleation sites

- Fifth line (possible):

n_dot - nucleation rate

dt - maximum time step allowed due to the precipitate condition

- Last line:

+ nucleation of CEMENTITE_P0 started at 0,00152588 s, T=600 °C (873,16 K) - Additional information: Nucleation started '+' or stopped '-' and the exact system parameters at that time.

Another output result, at a later stage:

```
******** isothermal, T=873.16 K (600 C)
**********************************************************
2500, recs=299; its=1/1, dt=0.000118979, time: 16.993s (0.00472h), T=600 C
(873.2 K), on Tue, 17:49:51
#Ferrite: BCC_A2, sv=6.13e-010 (sve=6.13e-010), dcf=1 (dt=0.099, matrix(C))
FE +9.99773e-001(+0.00e+000) C +2.27191e-004(+0.00e+000)
——————————————————————————————————
CEMENTITE_P0: (250/..gs/1e+020/d) f=0.03605/rm=3.85e-008/dfm=62.0,nucl-
dfm=62.0, ans=0
n_dot=0e+000 (ecdf=0.99), mcomp(its:0)=1 (res=0), step: (dt=2.4e-005, rad-
shrink/249)
```

In iteration 2500 above, the maximum time-step is set to **0.099** s to avoid the C content from being depleted too fast **(matrix(C))**. The carbon content of the matrix has decreased from **9.2×10^{-3}** initially (iteration 1) to **2.3×10^{-4}** in iteration 2500. The precipitate phase uses **250** classes and consists of roughly **1×10^{20}** particles. The mole fraction of cementite in the matrix is **0.0361** (3.61%). There is a small positive driving force for nucleation (**62.0 J**) and the nucleation rate (**n_dot**) is zero. This is because all nucleation sites are saturated (**ans=0**).

To avoid numerical instability, unreasonably large changes, for example in composition, precipitate volume, precipitate number or driving force, are prevented. Here, the coarsening stage is in progress and small particles are shrinking. A maximum value of radius reduction per time-step is imposed (**rad-shrink**); this reduces the time-step to **2.4×10^{-5}** s for the next step. The calculation speed can be increased by setting the windows to **'manual update'** so

that the graphs are not updated. Select **'View-Freeze update'** or press **'Ctrl+I'** to freeze the currently selected window. The same procedure unlocks the window again. To update the window content, press **'Ctrl+U'** or select **'View-Update all window contents'**.

INTERPRETING THE RESULTS

NUCLEATION, GROWTH AND COARSENING

When the calculation is finished, add three new plots in the same window as the plot of F$CEMENTITE_P0 versus time. Drag and drop **NUM_PREC$CEMENTITE_P0** (number of cementite precipitates) into the first of these, **NUCL_RATE$CEMENTITE_P0** (nucleation rate) into the second. In the third, add **R_MEAN$CEMENTITE_P0** (mean radius), **R_CRIT$CEMENTITE_P0** (critical radius), **R_MIN$CEMENTITE_P0** (minimum radius) and **R_MAX$CEMENTITE_P0** (maximum radius).

These variables can be found under **'kinetics: precipitates'** and **'kinetics: nucleation'** in the **'variables'** window. Using these plots, the different stages of nucleation, growth and coarsening can be identified.

During the **nucleation** stage, between 1e-11 and 1e-9 hours, the number of precipitates increases rapidly, but since these precipitates are, as yet, extremely small, the phase fraction of cementite also remains small. During this stage, the nucleation rate rises initially, due to a positive driving force for nucleation, and decreases again to zero when all the available nucleation sites are occupied.

The next stage, from approximately 1e-9 to 1e-6 hours, is the diffusion-controlled **growth** of these nuclei; this continues until the equilibrium phase fraction of cementite reaches its equilibrium value, as indicated by the plateau on the **'Phase fraction'** curve. The number of precipitates does not change during this stage, but there is an increase in radius which can just be detected on the plot below. There follows a period in which there is little or no change in any of the three parameters.

Finally, at just over 1e-3 hours onwards, there is the onset of **coarsening**, which is characterised by a decrease in the number of precipitates accompanied by an increase in radius. The critical radius rises and becomes larger than the smallest precipitate classes. Therefore these classes start to dissolve and the newly available carbon is used to grow the larger precipitates (Gibbs-Thomson effect). The minimum radius is unstable (leading to a 'noisy' appearance on the graph) as the small precipitates are shrinking (minimum radius goes down) and dissolving (minimum radius goes up to the next smallest class present in the system).

Phase fraction of cementite precipitate
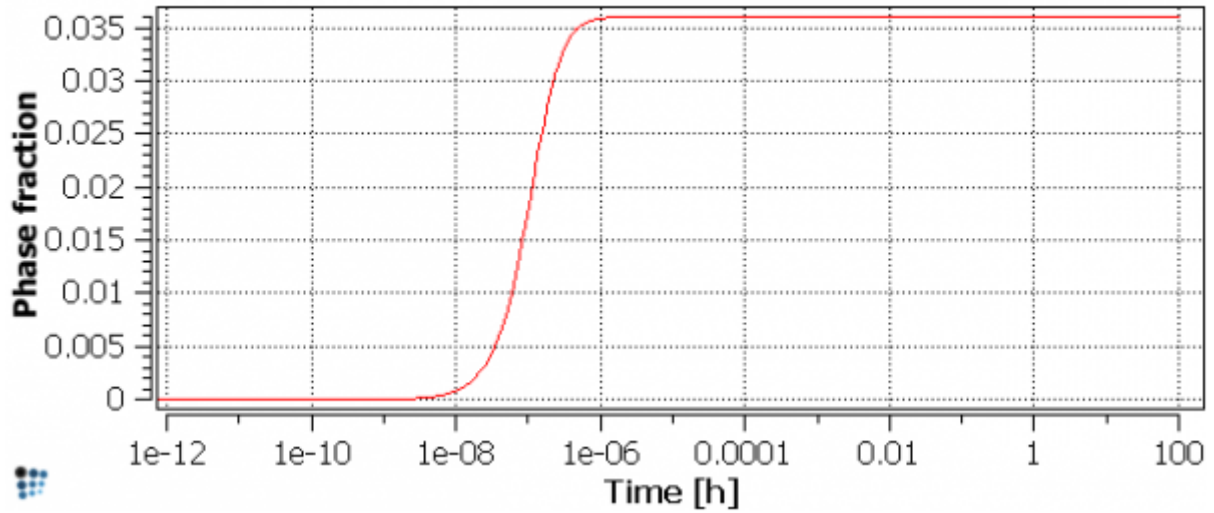
Number of precipitates

Nucleation rate
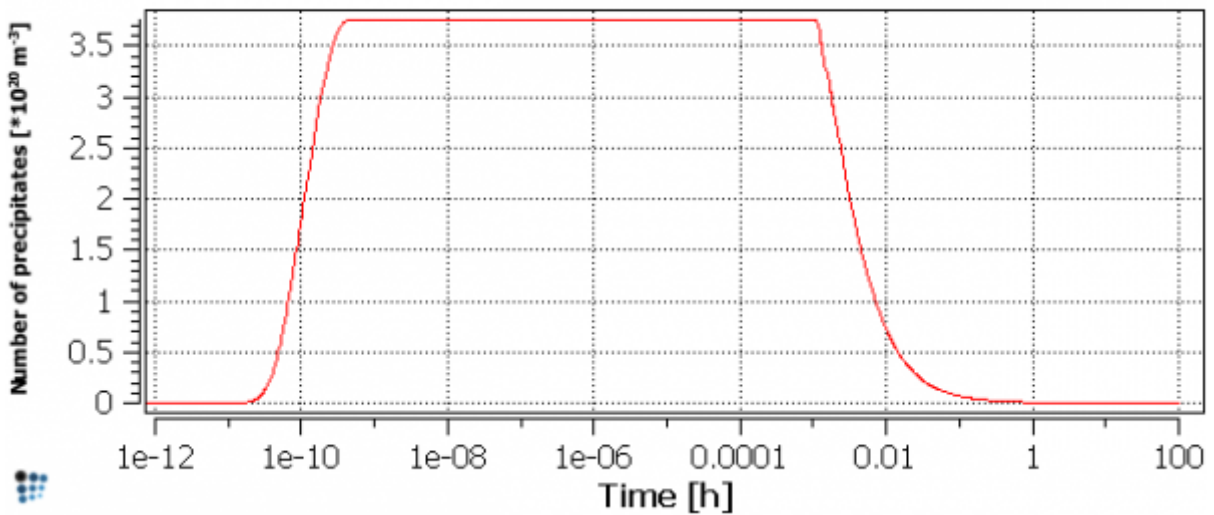
Precipitate radius
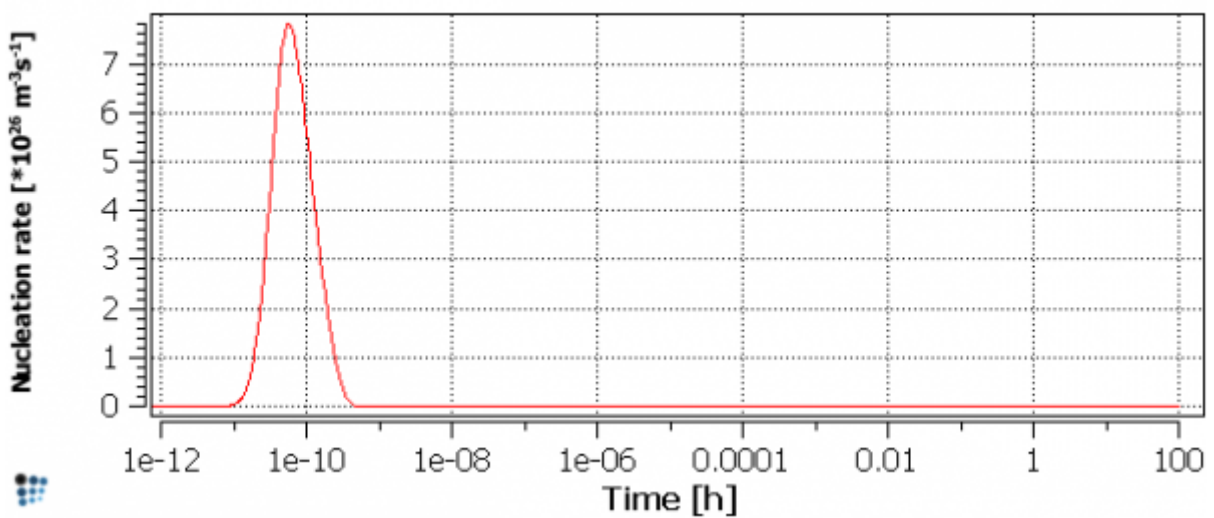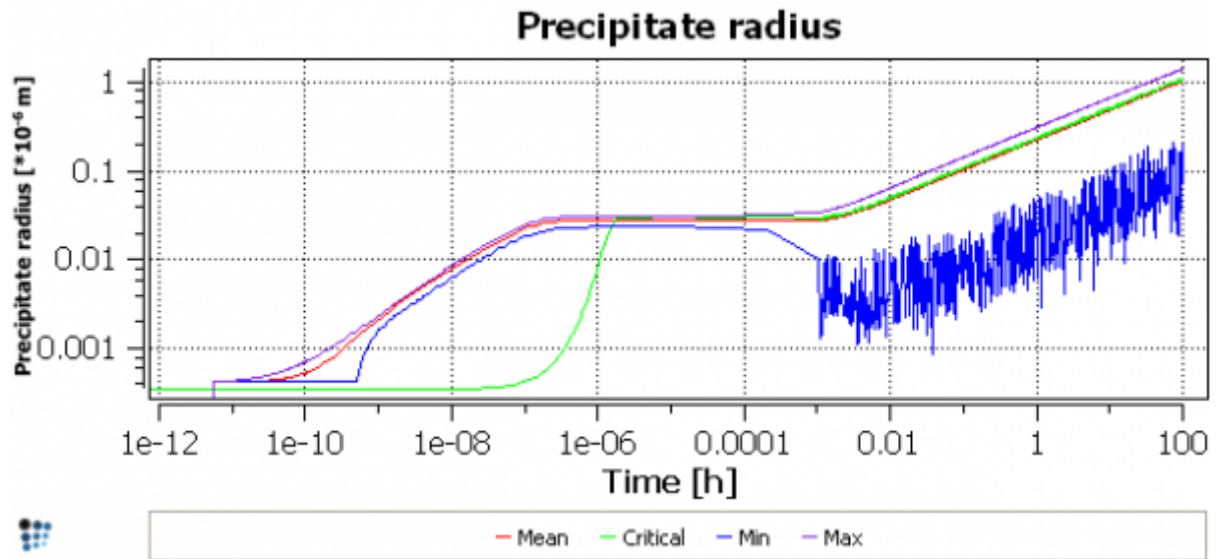
HISTOGRAMS OF PRECIPITATE SIZE DISTRIBUTION

The plot above shows only the variation of the mean radius with time, but more detailed information on the distribution of particle sizes can be found on the histogram. At the end of the calculation, the final size distribution is shown on the histogram. The distribution at other stages of the calculation can be recalled using **'Global > Buffers > Edit buffer states'**. This brings up a list of all the states saved in the memory, with details of time, temperature and time-step. Selecting one of these records loads the corresponding particle size distribution into the histogram if the **'auto load'** box at the bottom left is ticked. Otherwise, it can be loaded by clicking on the **'load selected'** button.

Cementite precipitate distribution
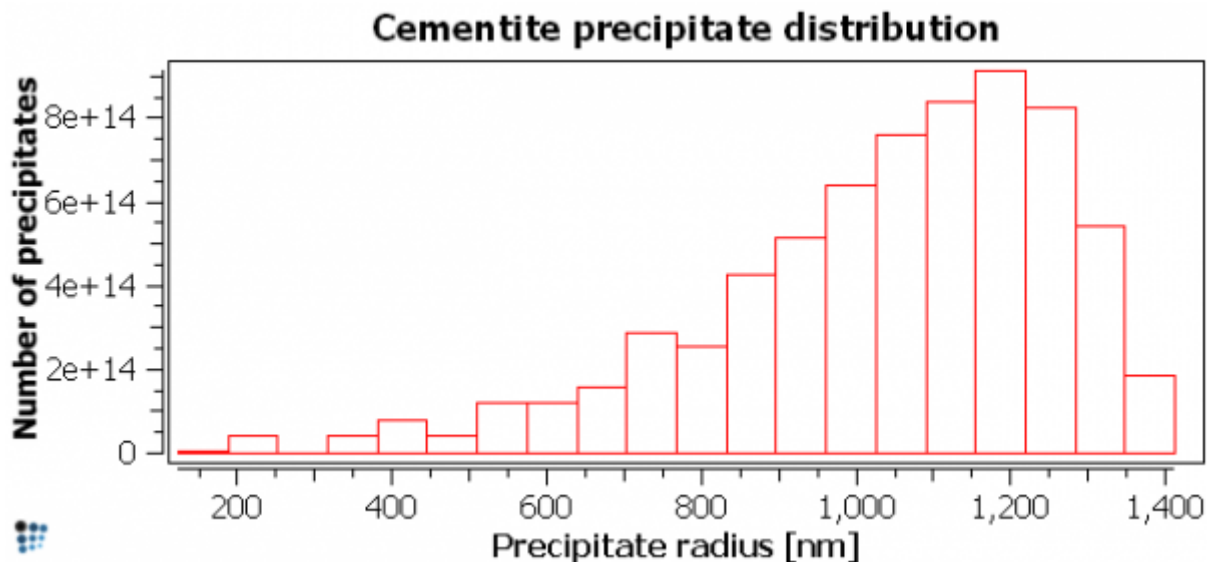
In the final part of this tutorial, the precipitate size distribution as calculated by MatCalc will be compared with the Lifshitz-Slyozov-Wagner (LSW) distribution given by the following equation:

$$f(x)=x^2 \cdot \left(\frac{3}{3+x}\right)^{\left(\frac{7}{3}\right)} \cdot \left(\frac{\frac{3}{2}}{\frac{3}{2}-x}\right)^{\left(\frac{11}{3}\right)} \cdot e^{\left(-\frac{x}{\frac{3}{2}-x}\right)} \cdot \frac{4}{9}$$

Create a new plot in the histogram window for CEMENTITE_P0 and set the number of classes on the histogram to 20 as before. In the options under **'plots'**, select **'density'** for **'scale frequency'** and **'yes'** for **'scale radius'**. Set the scaling of the x-axis as **'0..1.499'** because the LSW function is only defined between 0 and 1.5.

▼plots

↘ plot #0	id=02
title	Scaled cementite precipit...
# size classes	20
histogram type	number ▲▼
scale frequency	density ▲▼
scale radius	yes ▲▼
▶legend	
▼axes	

Enter the LSW function, either using the **'Functions and Variables'** box or by using the following command-line in the console:

```
set-function-expression LSW x^2*(3/(3+x))^(7/3)*((3/2)/(3/2-x))^(11/3)*exp(-
x/(3/2-x))*4/9
```

Then add the function to the scaled plot, either using the right-click menu in the Options window to add a new **'function/expression'** series (as it was done in Tutorial 6) or by using the following command-line:

```
set-plot-option . s n f LSW 0..1.5
```

The plot below shows a comparison between the LSW function and the histogram simulated by MatCalc.

Scaled cementite precipitate size distribution
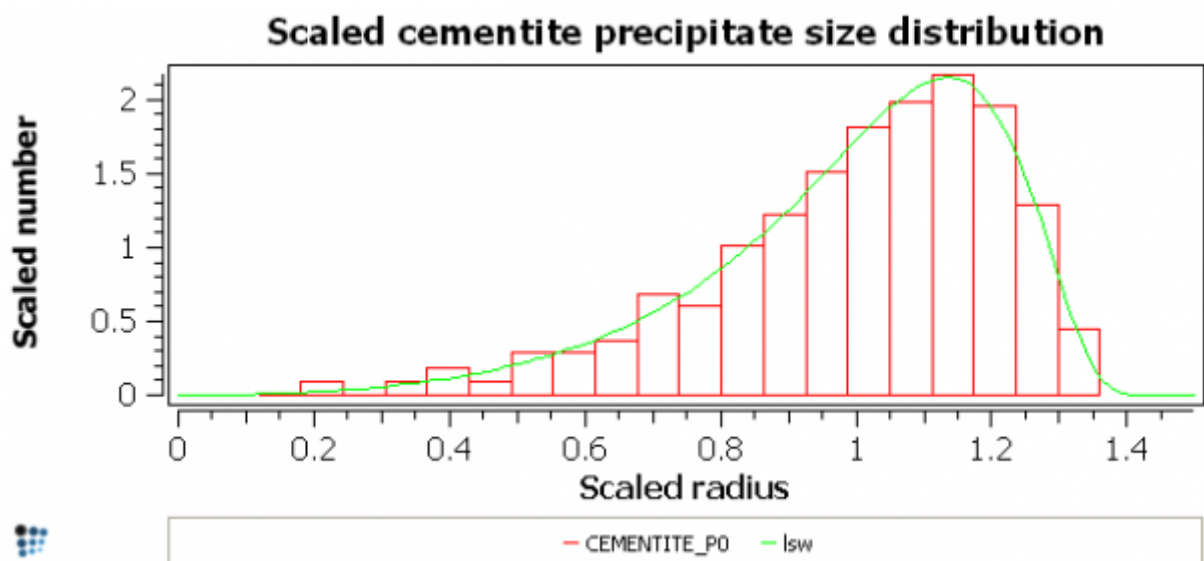
CONSECUTIVE ARTICLES

The tutorial is continued in article T15 - Effect of microstructure and conditions (Part 1)

T15: EFFECT OF MICROSTRUCTURE AND CONDITIONS (PART 1)

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb; mc_sample_fe.ddb

The Fe-Cr-C system forms the basis of many industrially useful alloys. The aim of this and Tutorial 16 is to produce a simulation of the precipitation behaviour in a Fe-10Cr-0.1C (wt.%) alloy during heat-treatment at 600°C. This involves considering several aspects, such as the chemical compositions of nuclei, the microstructural sites on which nuclei form, and the density of these sites in the microstructure under consideration. This first of two tutorials will focus on modelling the formation of the metastable cementite (Fe_3C) phase, and Tutorial 16 will consider the interaction between this and the more stable phase $M_{23}C_6$.

CONTENTS:

- Choice of nucleation model
- Diffusivity in precipitates
- Nucleation sites for the precipitate phase
- Microstructural parameters of the precipitation domain

EQUILIBRIUM CALCULATIONS

Create a new workspace with the elements Fe, C and Cr and the phases BCC_A2, CEMENTITE and M23C6. Enter the composition 10 wt.% Cr, 0.1 wt.% C.

Calculate an equilibrium at 600°C and observe the contents of the **'Phase summary'** window. It can be seen that $M_{23}C_6$ is the stable phase at equilibrium. However, it is known from experience that the first phase to form on heat-treatment is cementite.

Go to **'Global > Phase status'** and suspend the **'$M_{23}C_6$'** phase so as to study the metastable equilibrium between BCC_A2 and cementite. The composition of cementite in metastable equilibrium with BCC_A2 is, in wt.%, 85 % Cr, 7 % C, 8 % Fe; this is very rich in Cr compared to the overall system composition of 10 % Cr, 0.1 % C and 90.1 % Fe. Moreover, in the **'Phase summary'** window, a tag **'*maj!*'** appears next to the cementite phase which is a sort of MatCalc warning - after all, it is iron rather than chromium which is expected to be a major constituent in cementite

In practice, it is found that cementite forms rapidly on heat-treatment at 600°C; this is more consistent with a mechanism which primarily involves the diffusion of C rather than the slower-diffusing Cr. It is therefore likely that the initial nuclei do not form with the equilibrium composition, but are initially much richer in Fe than Cr. Part 1 of this tutorial considers how such effects can be modelled. Re-open **'Global > Phase status'** and remove the **'suspended'** flag for $M_{23}C_6$.

NUCLEATION MODEL FOR CEMENTITE

SETTING UP THE SIMULATION

Create a precipitate phase **CEMENTITE_P0**, using **'Global > Phase status'**. In the **'Precipitate'** tab, set the number of size classes to **'25'**, and in the **'Nucleation'** tab, change the **'Nucleus composition'** model from **'ortho-equilibrium'** to **'para-equilibrium'** using the drop-down menu. **'Para-equilibrium'** means that the nucleus is assumed to have the same composition in terms of substitutional elements as the matrix from which it forms, and only the carbon is partitioned between the two phases. In the **'ortho-equilibrium'** model, by contrast, the composition of the nucleus is calculated assuming full equilibrium with the BCC_A2 matrix. In the **'Nucl. sites'** tab, set the nucleation sites to **'Dislocations'** (remove the tick from 'bulk')
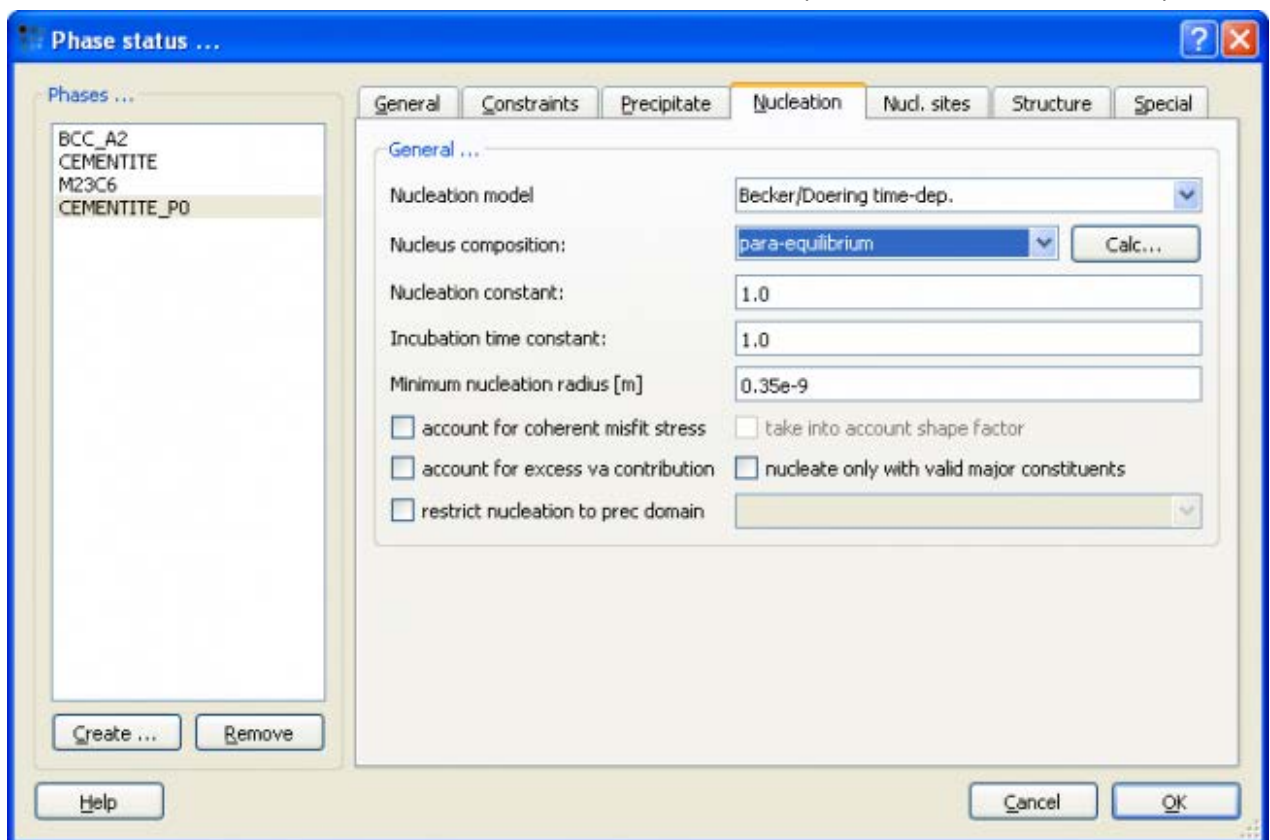
In **'Global > precipitation domains'**, create a new domain named **'ferrite'** with **'BCC_A2'** as its matrix phase. Click on **'Attach'**, select **'CEMENTITE_P0'** and click **'OK'**. The system is now set up so that cementite can precipitate in this domain. Accept the changes by clicking **'OK'** to close the window.
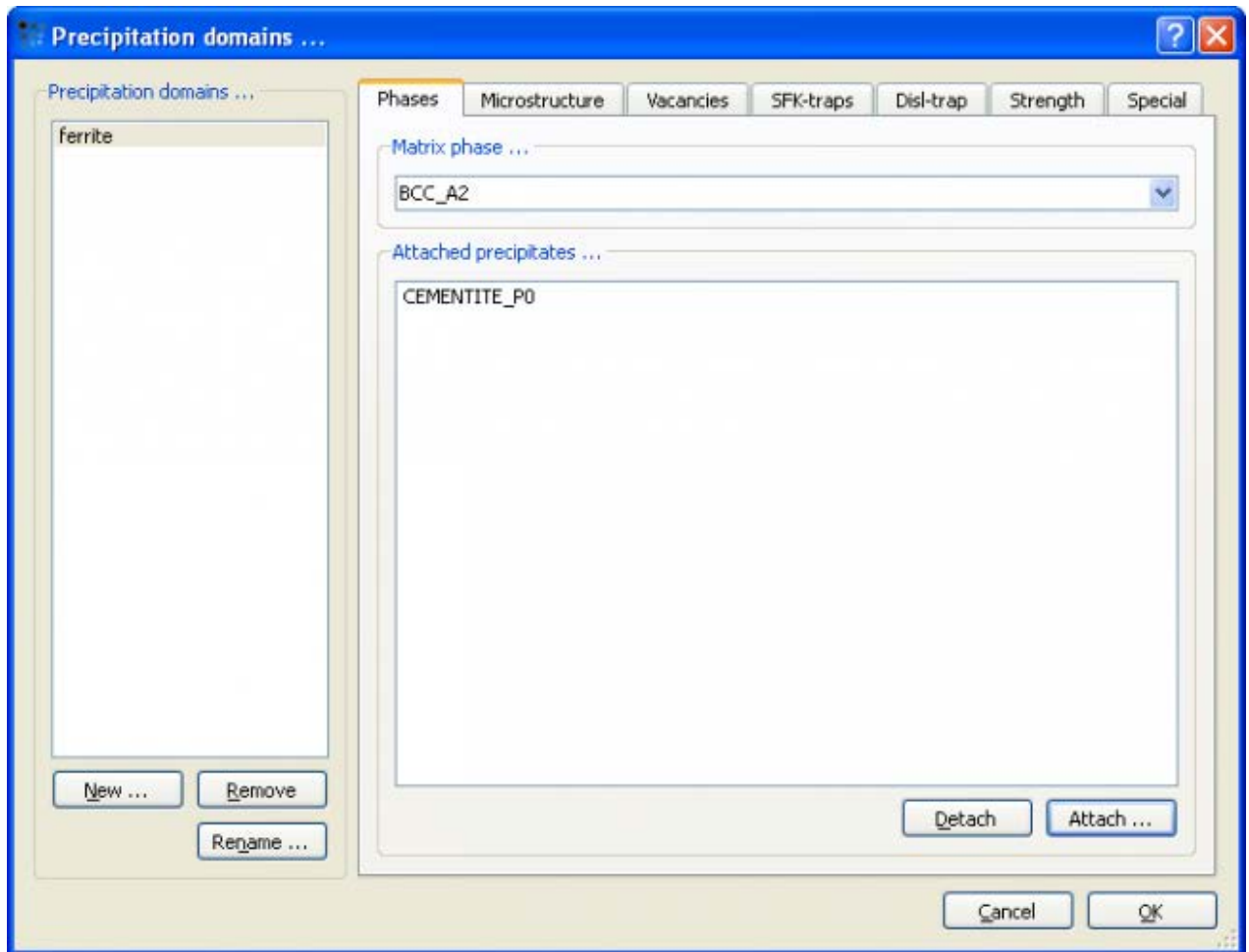
Load the mobility data as described in Tutorial 14.

GRAPHICAL DISPLAY OF RESULTS

Create a new XY-plot window and define a default x-axis with the following properties:

- **Use for all plots**: yes
- **Title**: Time [h]
- **Type**: log
- **Scaling**: 1e-10..
- **Factor**: 1/3600 (to convert seconds to hours)

Add four new plots to the window and drag and drop the following series to the plots:

1. **F$CEMENTITE_P0**
2. **X$CEMENTITE_P0$CR** (Cr content of the cementite precipitate phase) and **X_NUCL$CEMENTITE_P0$CR** (Cr content of the nucleus). The latter can be found under **'kinetics: nucleation'**.
3. **XBCC_A2C** (carbon content of BCC matrix)
4. **NUM_PREC$CEMENTITE_P0**
5. **R_MEAN$CEMENTITE_P0**

Label the y-axes as follows

1. **'f_{CEM}'** (f_{CEM})
2. **'x_{Cr}'** (x_{Cr})
3. **'x_{BCC_A2, C}'** ($x_{BCC\_A2, C}$)
4. **'N_{ppt}[m⁻³]'** ($N_{ppt}[m^{-3}]$)
5. **'R_{mean} [m]'** (R_{mean} [m]); y-axis set to **'log'**

Save the workspace.

CALCULATION

Select **'Calc > precipitate kinetics'**. Enter the finish time of the calculation: **'3.6e13'** s (= 1e10 hours). The isothermal treatment temperature should be set to **'600'** and **'Temperature in C'** selected. Leave the other settings as they are, and click on **"Go"**. (The calculation may take some time, especially on slower machines, because of the long treatment time.)

After the calculation has finished, duplicate and lock all the series in the plot window. Return to **'Global > Phase status'** and set the nucleation model for CEMENTITE_P0 to **'ortho-equilibrium'** and re-open **'Calc > precipitation kinetics'**. There is no need to change anything; simply click on **'Go'**. A warning appears that the contents of the current buffer will be overwritten. As the series have been locked, this does not matter; accept the warning with **"Yes"**.

INTERPRETATION OF RESULTS

The onset of precipitation occurs much earlier in the para-equilibrium case, beginning around 1e-7 hours (~ 1e-3 seconds), as compared to ~1 hour for ortho-equilibrium. The para-equilibrium cementite fraction reaches a plateau at a smaller value than for the ortho-equilibrium case, but after a longer time at temperature, this fraction rises, eventually reaching the same value as for ortho-equilibrium.
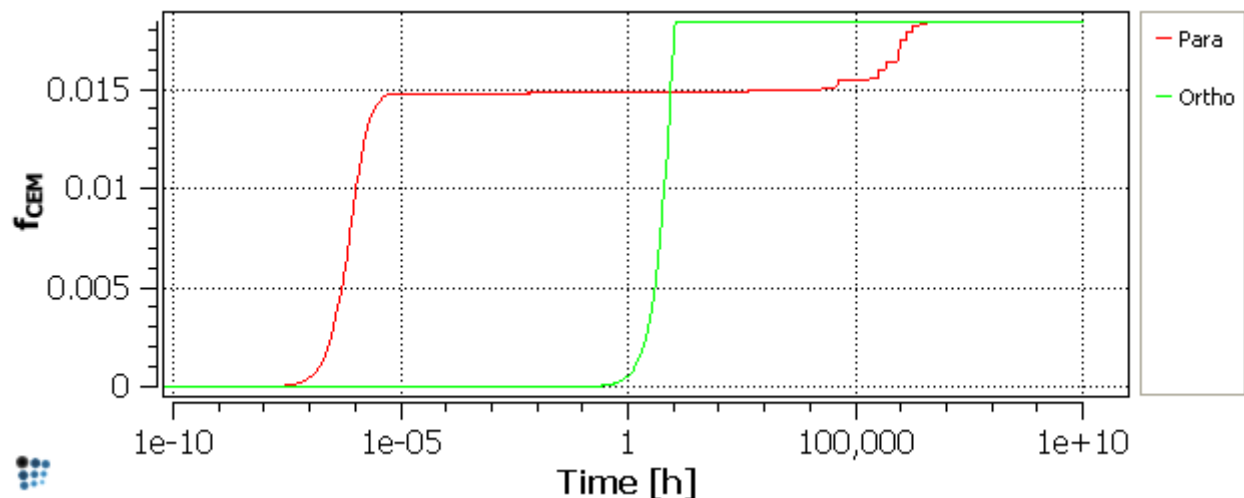
The para-equilibrium model stipulates that the Cr content of the nuclei ($x_{NUCL,CEM}$, Para) be equal to that of the matrix. This decreases towards longer times at temperature, as the matrix

becomes depleted in Cr. This depletion is caused by the Cr-enrichment of the precipitates by diffusion; their Cr content (X_{CEM}, Para) increases up to the equilibrium value of around 0.69 (mol. fr.).

In the ortho-equilibrium case, the cementite nucleates with its equilibrium Cr content, and there is little or no change in the Cr content of the precipitates during the heat-treatment. It is this requirement for full equilibrium which accounts for the long incubation time for cementite when the ortho-equilibrium model is used; the formation of a critical nucleus with ortho-equilibrium composition requires the (slower) diffusion of Cr.
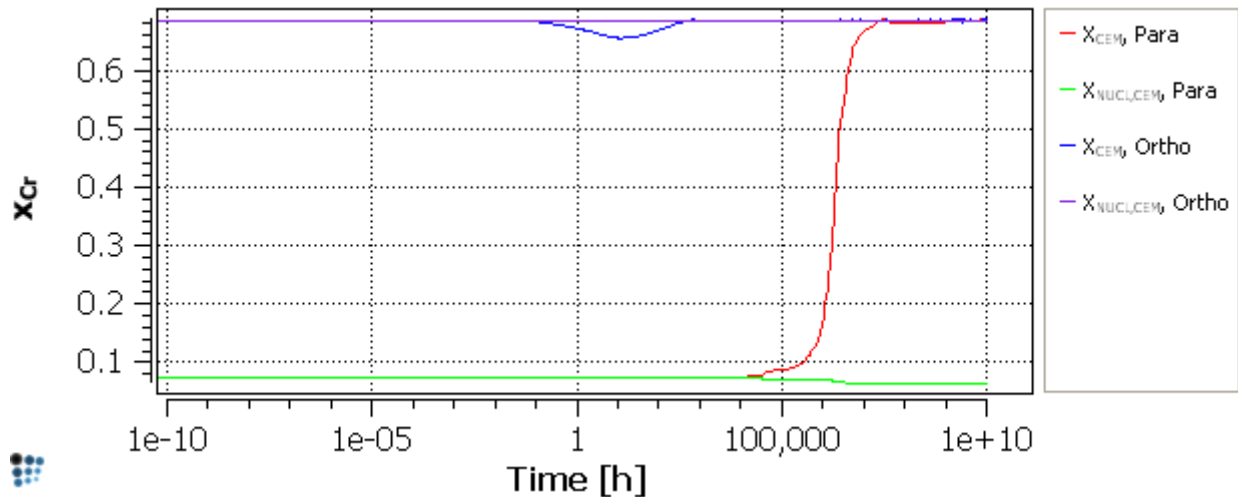
In the plot of XBCC_A2C (the carbon content of the BCC matrix), it can be seen that the depletion of the matrix in carbon exactly follows the increase in precipitate fraction for both models.
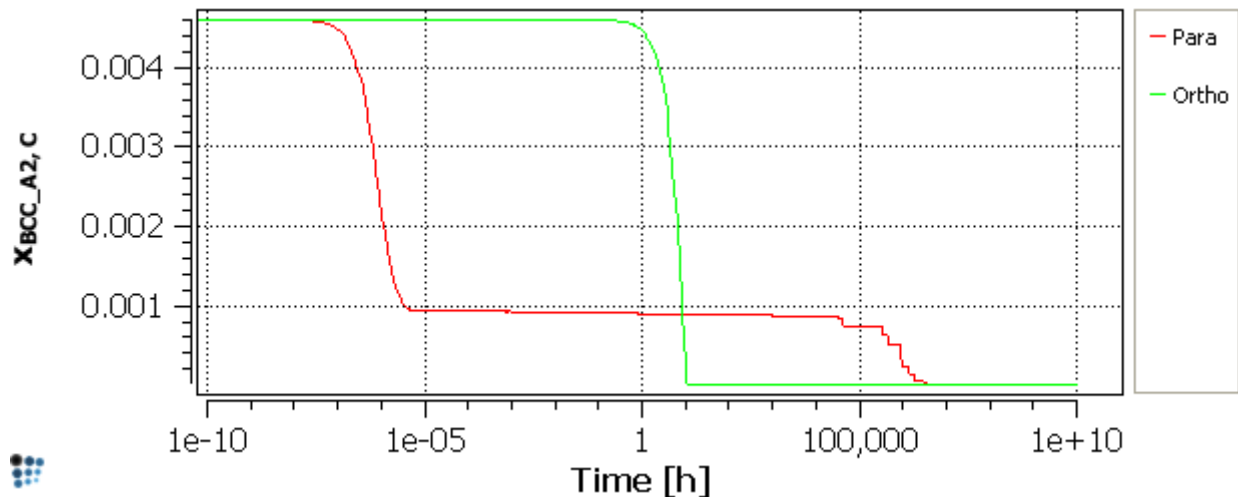
The plot of the number of cementite precipitates shows that in the ortho-equilibrium case, nucleation occurs at a later stage and the precipitates are less numerous.
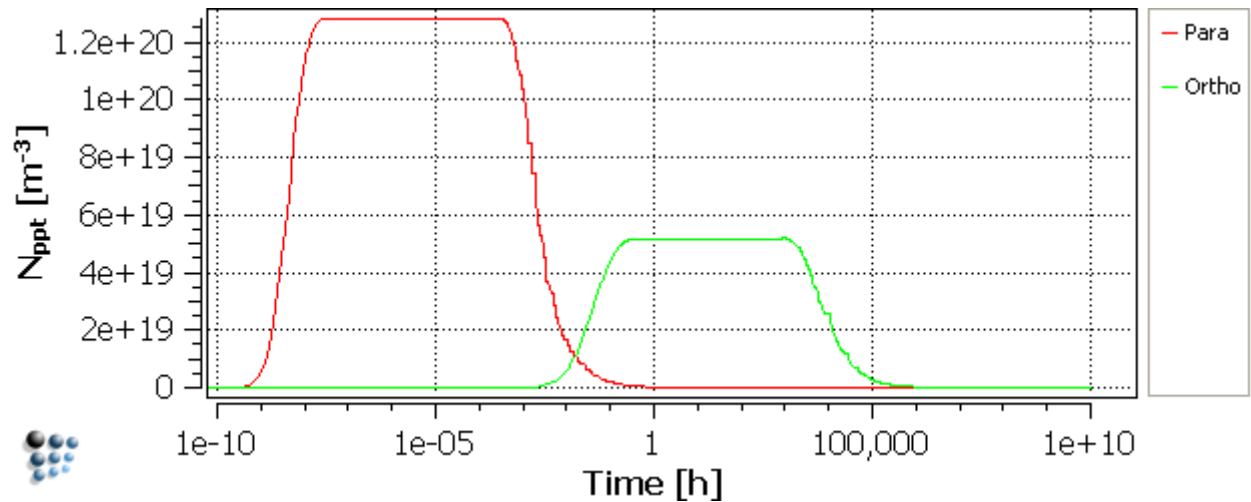
Coarsening of the precipitates is more rapid in the para-equilibrium case, as can be seen from the plot below:
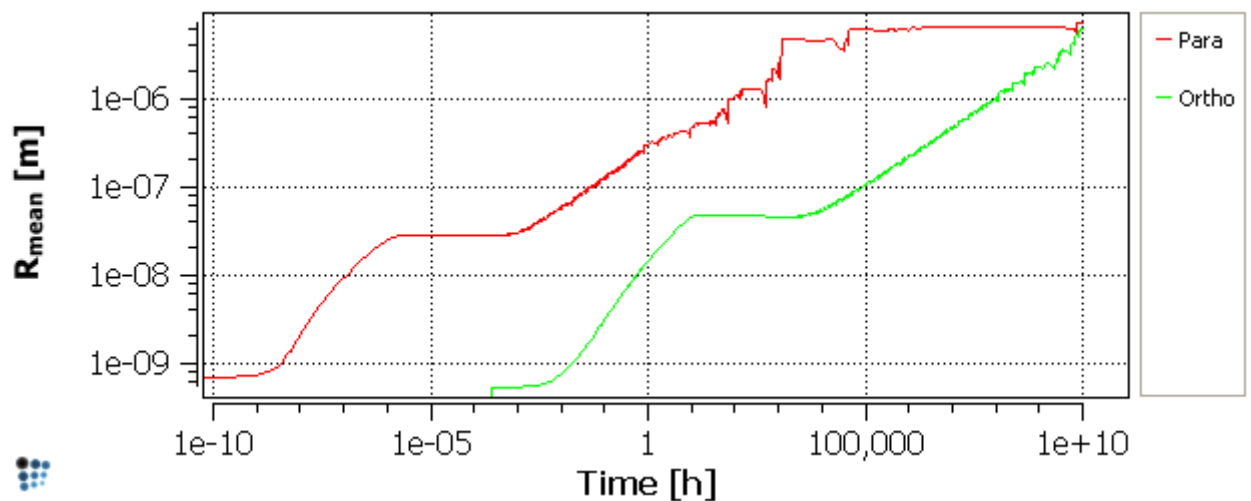
The use of the para-equilibrium nucleation model gives better qualitative agreement with experimental observations of the rapid precipitation of cementite at temperatures such as 600°C in alloy steels. An example in the Examples section, in which this issue is considered in more detail, will be available shortly.

DIFFUSIVITY IN PRECIPITATES

SETUP

It was seen above that, using the para-equilibrium model, cementite precipitates formed with a Fe-rich composition and subsequently enriched in Cr. The rate of enrichment depends on the ease with which chromium can diffuse into existing precipitates.

Duplicate and lock all the series in the plots. Re-open **'Global > Phase status'**. In the **'Nucleation'** tab, set the cementite nucleation model to back to **'para-equilibrium'**. Open the **'Special'** tab. In the **'Diffusion in precipitate as ratio from matrix …'** section, the selected

value of the **'substitutional'** ratio is set to 0.01. This means that the diffusivities of all elements within the cementite precipitate are considered to be one hundredth of their values within the matrix. Changing this value will affect the rate of Cr-enrichment of the cementite. To demonstrate this, change the value of the ratio to **'0.25'**, click on **'OK'** and re-run the simulation.
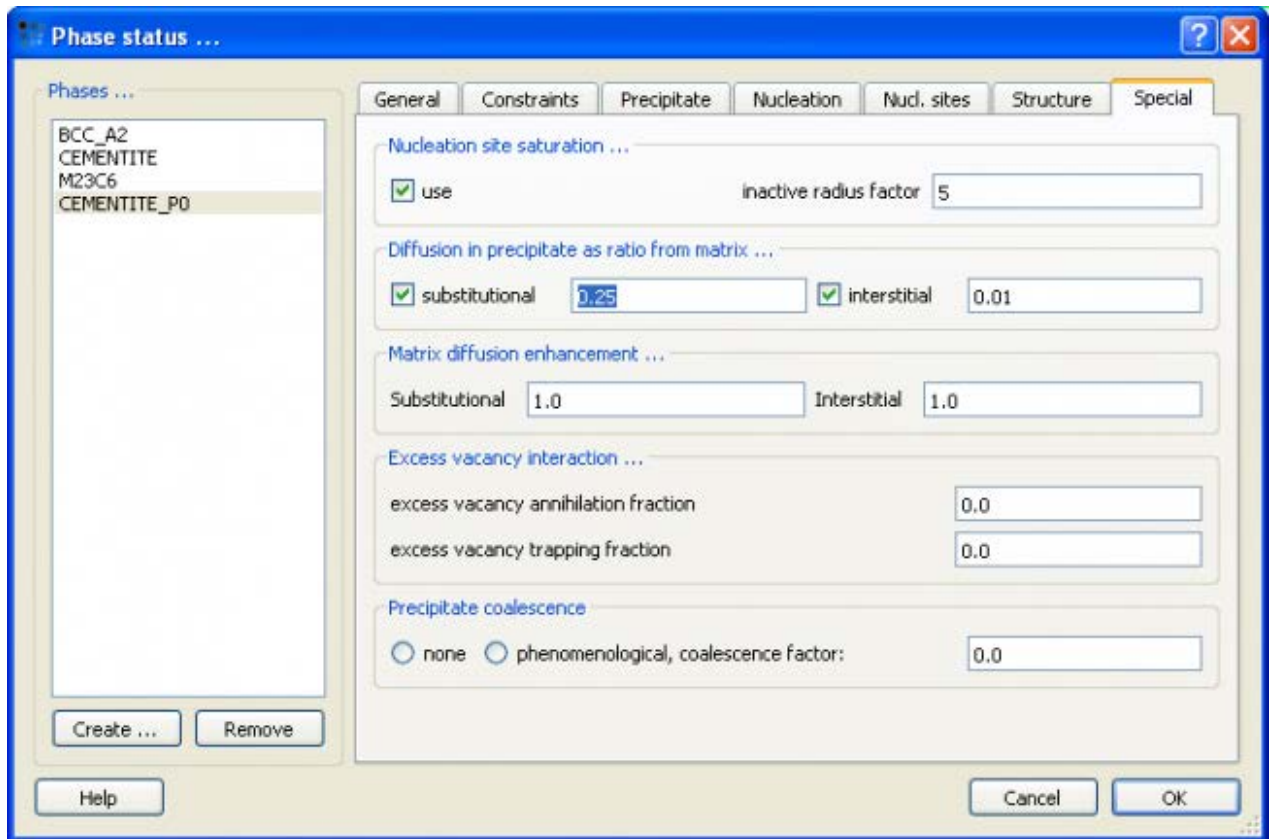
INTERPRETATION OF RESULTS

In this case, precipitation occurs at the same rate as in the first para-equilibrium calculation, but the Cr-enrichment of the precipitates is more rapid. Consequently, the increase in precipitate phase fraction and the decrease in matrix carbon content occur earlier.

It is also notable that coarsening is delayed and the distribution of more numerous, relatively fine particles is stabilised to longer times, as shown by the two plots below.
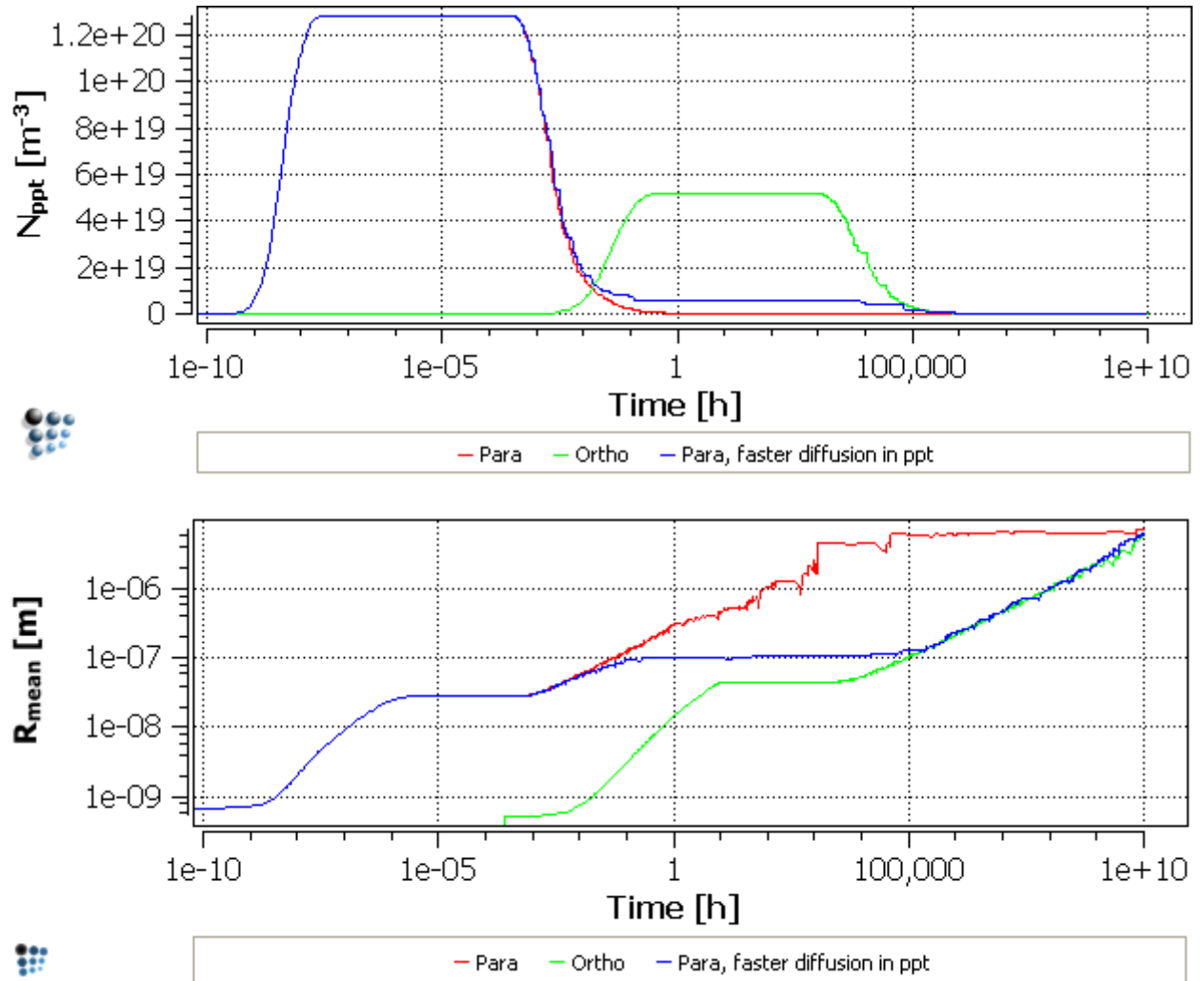
MICROSTRUCTURAL PARAMETERS AND NUCLEATION SITES

SETUP

At this stage, it may be helpful to remove all the series except the original para-equilibrium calculation results from the plots to avoid them becoming cluttered. (If required, the numerical data from the series can first be exported in text form using **'Copy data'** from the right-click menu and then pasting these data into a spreadsheet or text editor. Alternatively, the plots can be exported in graphical form using **'Copy pixmap'**.) To remove a series from a plot, first click on that plot and then select the name of the series in the **'Options'** window. (Failure to do this can result in series from other plots being deleted instead.) Multiple series can be selected using the Ctrl button. Remove them using the Delete button or **'Remove series'** from the right-click menu.

Reset the **'consider as ratio from matrix diffusivity'** value back to its default value of **'0.01'** in the **'Special'** tab, keep the nucleus composition model set at **'para-equilibrium'** and click **'OK'**

to save the changes. Open **'Global > precipitation domains'** and click on the **'Microstructure'** tab. The default values for each of the structural parameters are shown in the image below.
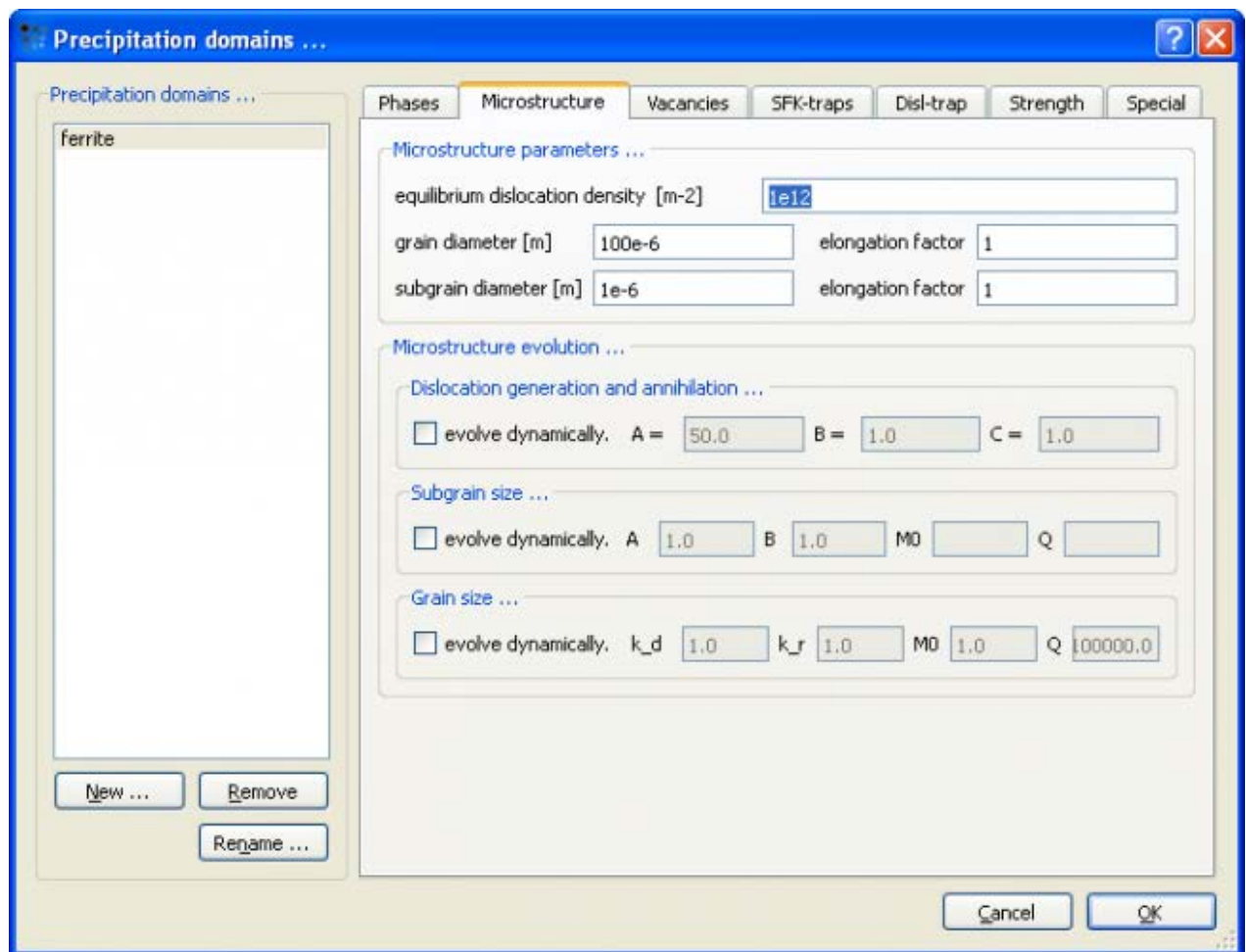
The nucleation sites for CEMENTITE_P0 have been set to **'Dislocations'** (see the section 'Setting up the simulation' of this tutorial) so the dislocation density will determine the number of nucleation sites. The default dislocation density, which has been used so far, is 1e12, which is typical of an annealed structure. Change this value to **'1e14'** and re-run the simulation.

The following images show the phase fraction, the number of precipitates (**note the log scale**) and the mean radius for dislocation densities of 1e12, 1e14 and 1e16. It can be seen that increasing the nucleation site density accelerates the reaction kinetics and results in a larger number of precipitates with a smaller mean radius.
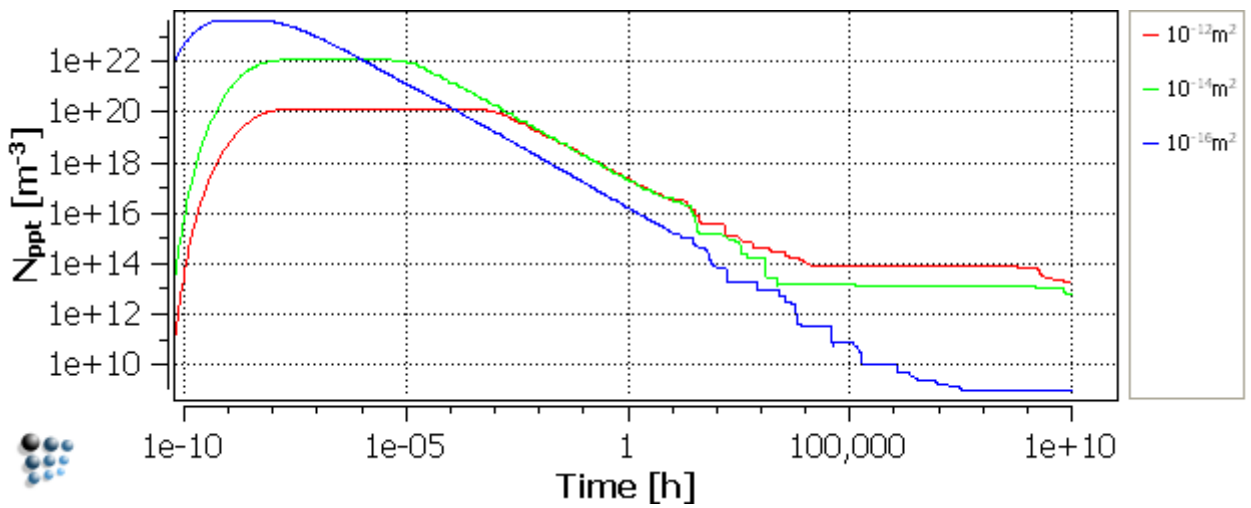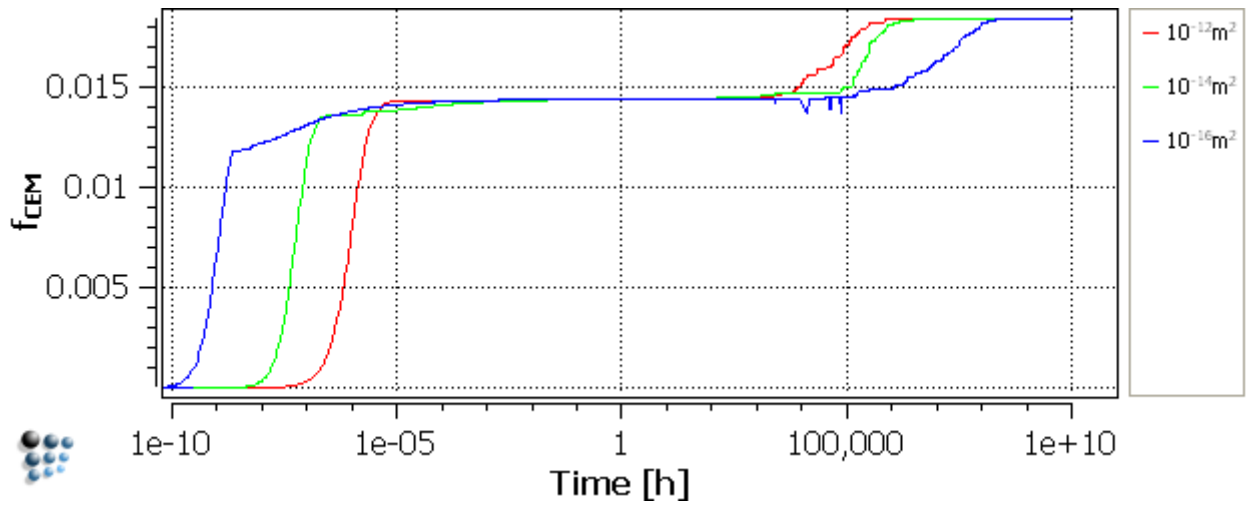
To finish…

Save the workspace file.

CONSECUTIVE ARTICLES

The tutorial is continued in article T16 - Effect of microstructure and conditions (Part 2 - simultaneous precipitation)

T16: Effect of microstructure and conditions (Part 2)

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb; mc_sample_fe.ddb

Contents:

- Simultaneous precipitation of two phases
- Effect of dislocation density
- Effect of grain diameter
- Subgrains and elongation factors

Before starting...

Re-open the workspace saved from Tutorial 15 and save it under a new name.

Simultaneous precipitation of cementite and $M_{23}C_6$

Setup

Open **'Global > Phase status'** and create a precipitate phase from $M_{23}C_6$. In the **'precipitate'** tab, enter **'25'** for the number of size classes, and attach the phase to the domain **'ferrite'**. In the **'Nucleation'** tab, set the nucleus composition model to **'ortho-equilibrium'**. Set the nucleation sites to **'Grain boundaries'** in the **'Nucl. sites'** tab.
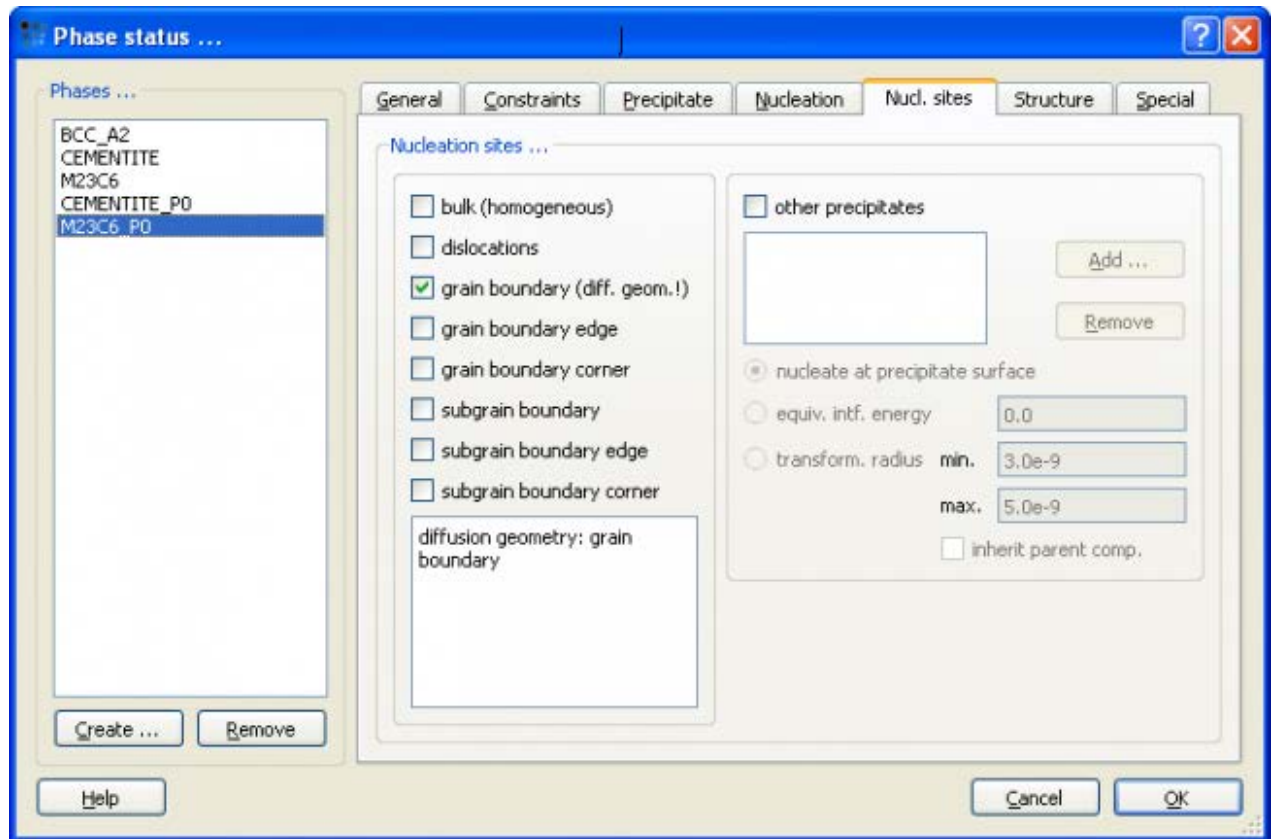
In **'Global > Precipitation domains > Microstructure'**, reset the dislocation density to its default value of **'1e12'** m^{-2}. The default grain diameter is **'100e-6'** m, and it is this which governs the density of M23C6_P0 nucleation sites. Modify the existing five plots to contain the following series:

1. **F$CEMENTITE_P0, F$M23C6_P0** (fraction of cementite and M23C6 precipitated, respectively)
2. **X$CEMENTITE_P0$CR, XBCC_A2CR** (Cr content of cementite precipitates and matrix, respectively)
3. **XBCC_A2C** (C content of matrix)
4. **NUM_PART$CEMENTITE_P0, NUM_PART$M23C6_P0** (number of cementite and M23C6 precipitates, respectively)
5. **R_MEAN$CEMENTITE_P0, R_MEAN$M23C6_P0** (mean radius of cementite and M23C6 precipitates, respectively)

Run the kinetic simulation, with an isothermal heat treatment at **600°C** as before, and an end time of **3.6e+10 s**.

INTERPRETATION OF RESULTS

Plot 1: Cementite appears rapidly and reaches a steady-state precipitate fraction. $M_{23}C_6$ starts to form after around 1 hour at 600°C; this is at the expense of cementite, which redissolves. By the end of the simulation, all the cementite has dissolved and $M_{23}C_6$ has reached its equilibrium phase fraction.
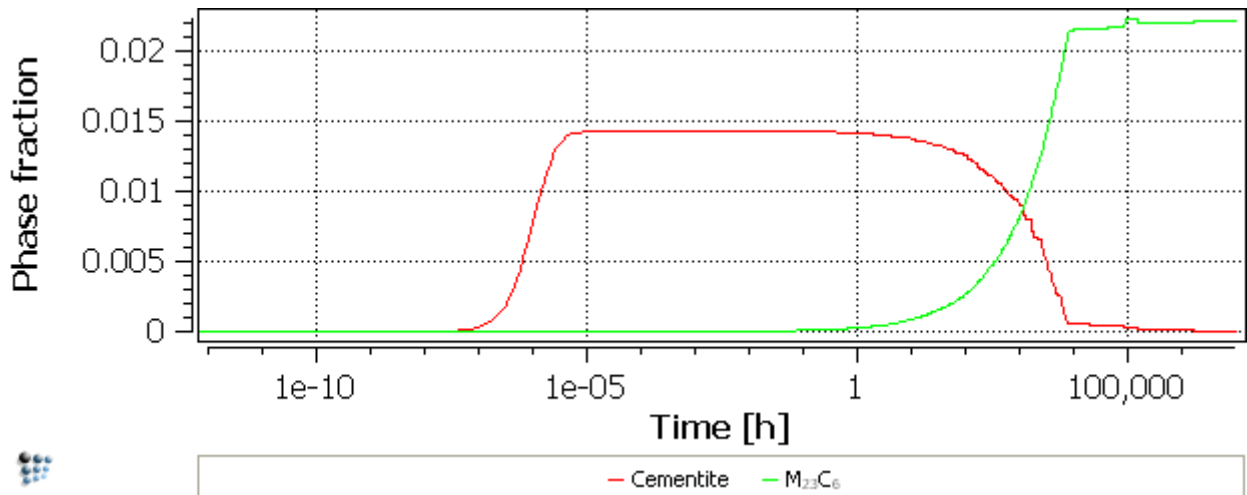
Plot 2: This shows that cementite enrichment has just started by the time the cementite phase is being dissolved.
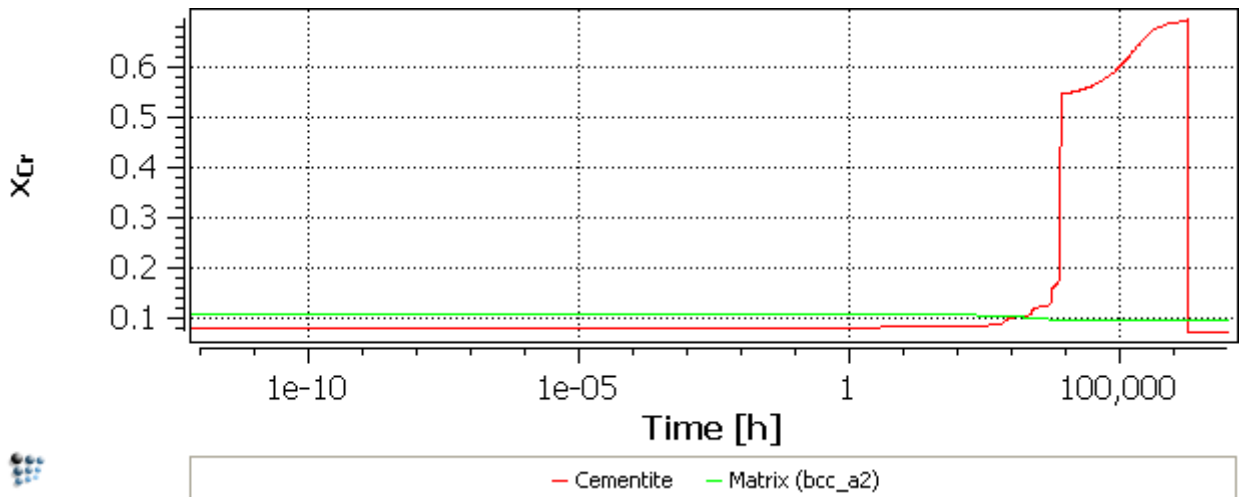
Plot 3: The depletion of the matrix in carbon occurs in two stages. The first of these corresponds to the formation of cementite, and the second to the formation of $M_{23}C_6$.
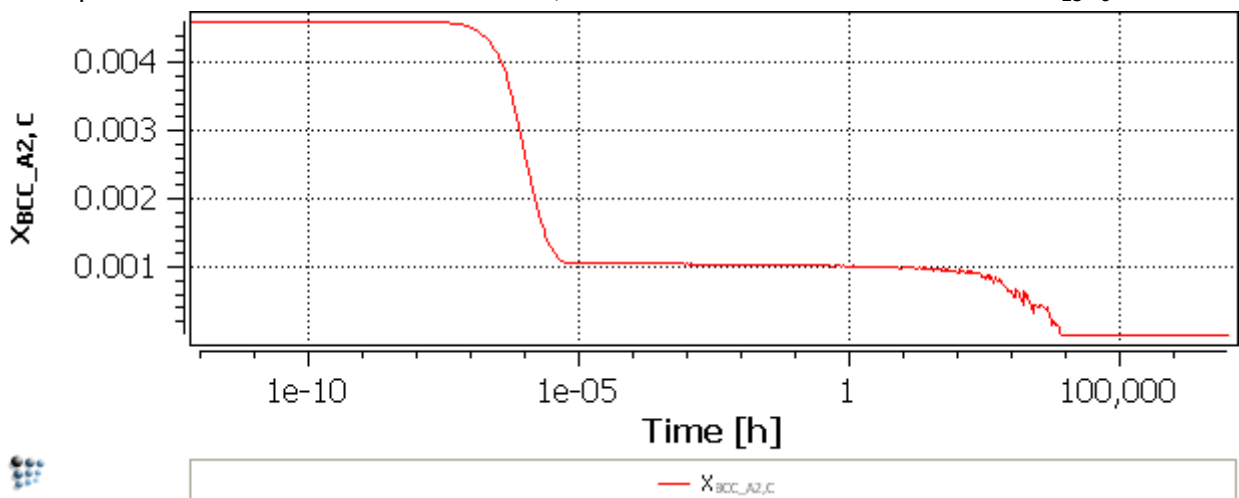
Plot 4: The number of $M_{23}C_6$ precipitates is comparable with that of cementite precipitates. The reduction in the number of cementite precipitates is both due to the coarsening and the phase dissolution stages:
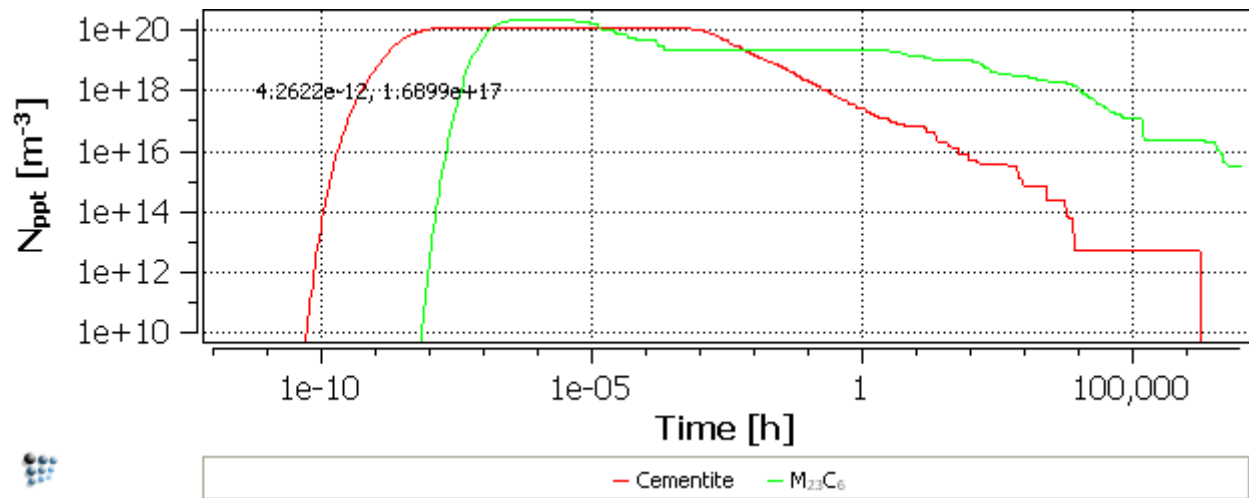
Plot 5: There is an intermediate stage between the growth and coarsening phases for the cementite precipitates (plateau between 10^{-6} - 10^{-3} hours). The maximal size of the cementite precipitates is in the micrometer range.
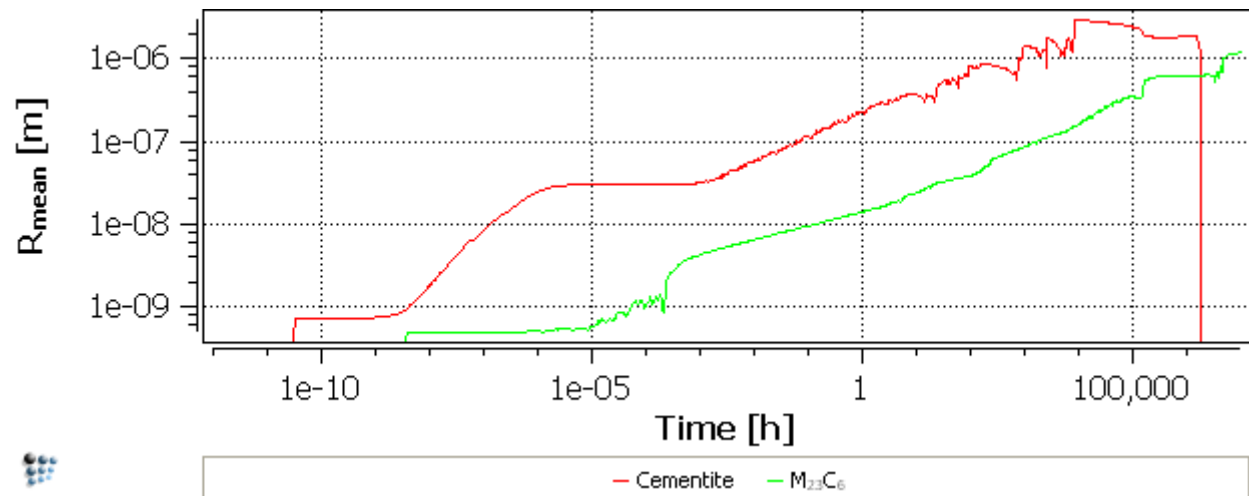
EFFECT OF DISLOCATION DENSITY

Duplicate and lock the series and re-run the simulation with a dislocation density of **1e14 m^{-2}**, leaving the grain size the same.

RESULTS:

The onset of cementite precipitation occurs earlier with a higher dislocation density, but the kinetics of cementite dissolution and of $M_{23}C_6$ precipitation are unchanged. The plot below shows a significant increase (note log scale) in the number of cementite precipitates formed.

Legend: — Cementite, $10^{12}m^{-2}$, 10^{-4} m   — $M_{23}C_6$, $10^{12}m^{-2}$, 10^{-4} m   — Cementite, $10^{14}m^{-2}$, 10^{-4} m   — $M_{23}C_6$, $10^{14}m^{-2}$, 10^{-4} m
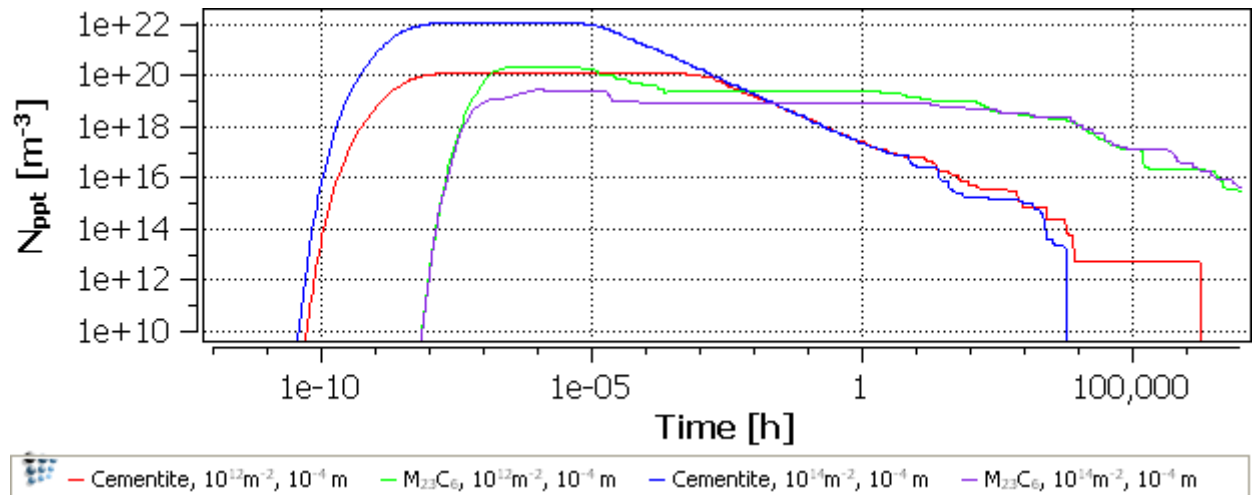
With a higher dislocation density, the cementite particles do not become so large during the growth stage. However, coarsening begins earlier, and the curve of radius versus time for the coarsening precipitates eventually becomes parallel with that for the lower dislocation density.

Legend: — Cementite, $10^{12}m^{-2}$, 10^{-4} m   — $M_{23}C_6$, $10^{12}m^{-2}$, 10^{-4} m   — Cementite, $10^{14}m^{-2}$, 10^{-4} m   — $M_{23}C_6$, $10^{14}m^{-2}$, 10^{-4} m
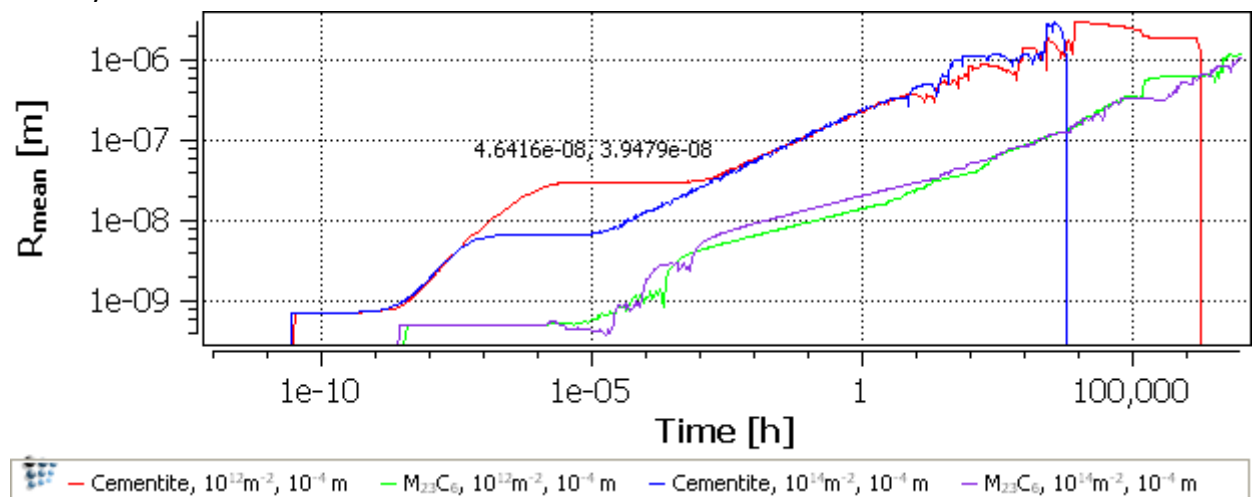
EFFECT OF GRAIN DIAMETER

Reopen **'Global > Precipitation domains > Structure'**. Reset the dislocation density to **1e12 m⁻²**, set the grain diameter to **10e-6 m** and re-run the simulation.
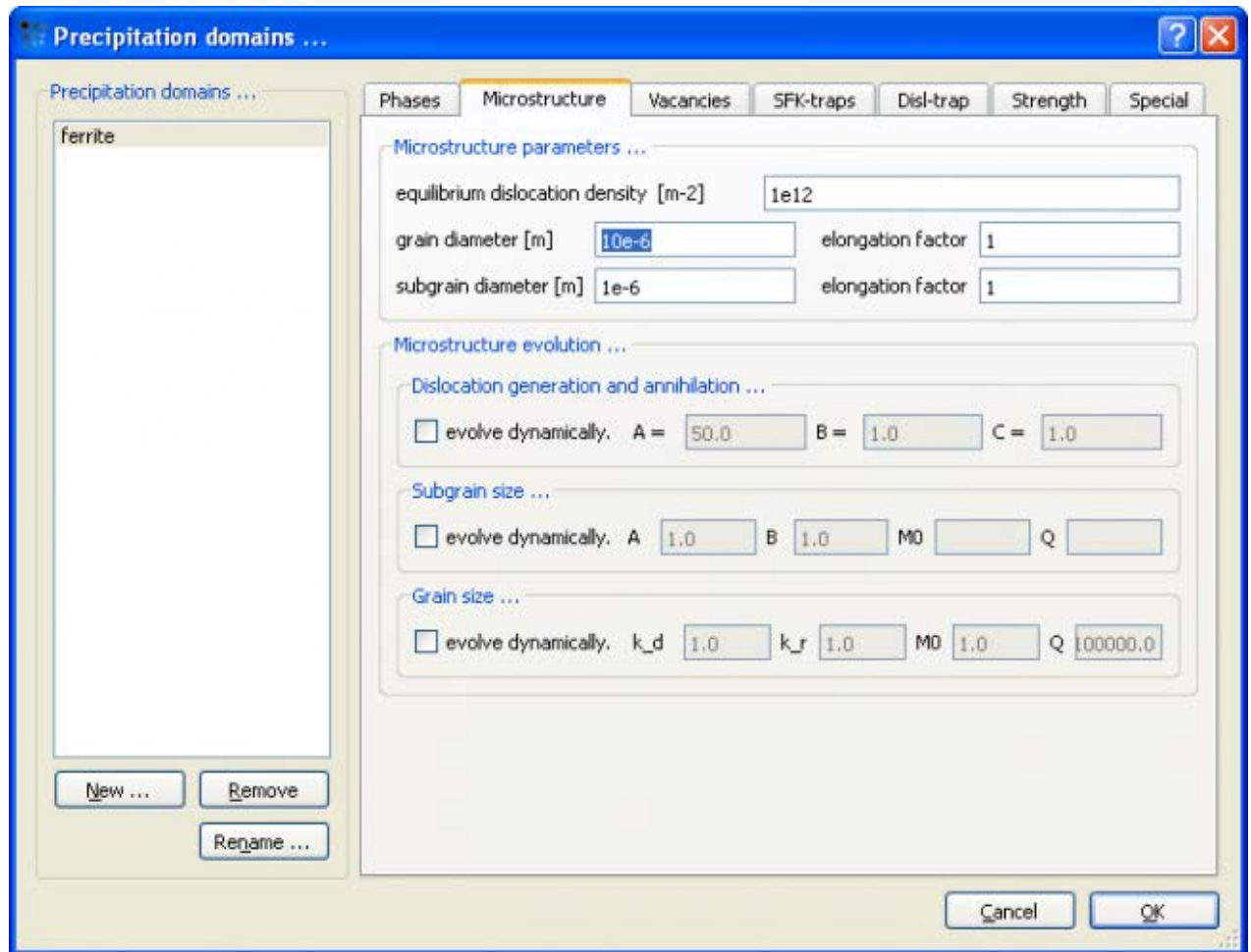
RESULTS:

As might be expected, reducing the grain diameter accelerates the precipitation kinetics of $M_{23}C_6$, by providing more nucleation sites. It also accelerates the dissolution of cementite, which begins to dissolve when $M_{23}C_6$ starts to precipitate.
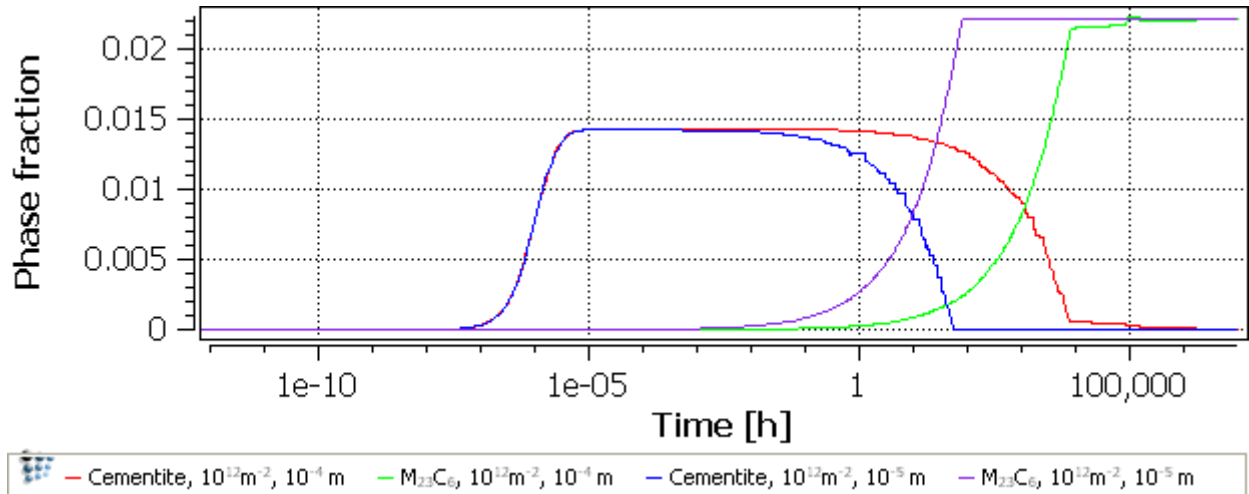
The plot below shows the effect on the number of $M_{23}C_6$ of reducing the grain size from 10^{-4} to 10^{-5} m. The number of $M_{23}C_6$ increased due to more nucleation sites available.
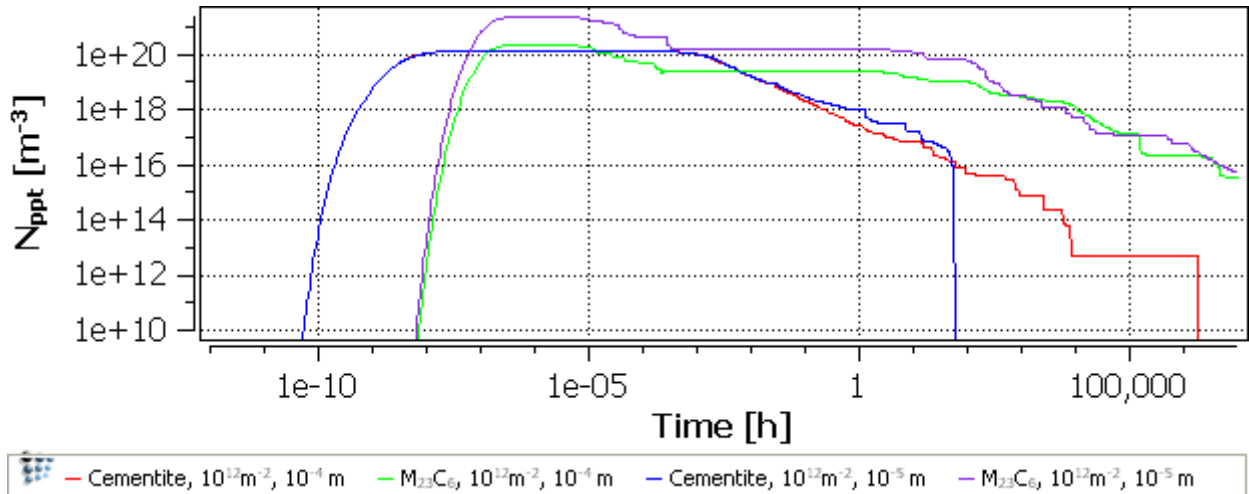
In the plot of radius against time, the maximum cementite radius attained is reduced, because there is less time available for coarsening of this phase before dissolution sets in.
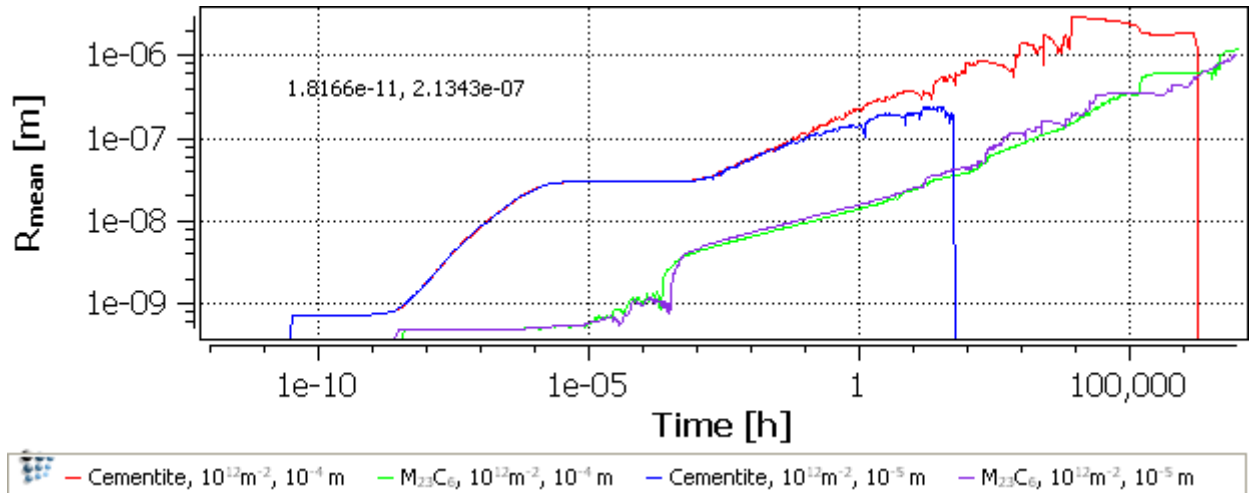
SUBGRAINS AND ELONGATION FACTORS

In the **'Global > Precipitation domains > Structure'**, the other adjustable parameters in the **'Microstructure parameters'** section are:

- **Grain size elongation factor**, i.e. aspect ratio of grains. This is useful in, for example, extruded structures, in which grains tend to be elongated in the direction of extrusion.
- **Subgrain diameter**. Subgrains are structures such as the packets and blocks of martensite in prior austenite grains, or polygonised structures formed during recovery of cold-worked materials. In the **'Global > Phase status > Nucleation'** tab, subgrain boundaries as well as grain boundaries, can be selected as nucleation sites.
- **Subgrain size elongation factor**: analogous to the grain size elongation factor, for subgrains.

Re-open **'Global > Phase status > Nucl. sites'**. In the **'Nucleation sites'** section select **'subgrain boundary'** in addition to **'grain boundary'** for M23C6_P0, to allow this phase to nucleate on subgrain as well as grain boundaries.
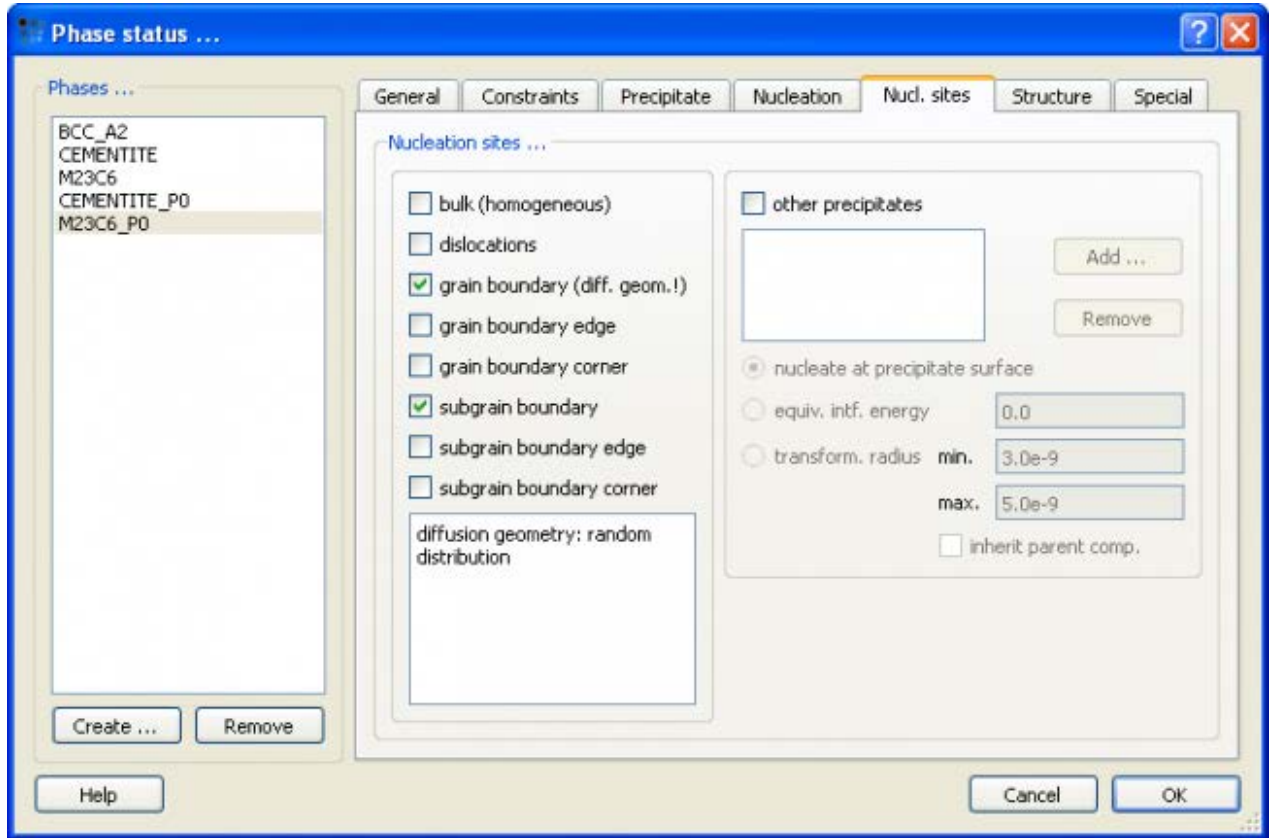
The default subgrain size in **'Global > Precipitation domains > Structure'** is 1e-6 m; accept this value and re-run the simulation.

The plots below compare calculations in which the dislocation density is **1e-12 m^{-2}** and the grain diameter is **10e-6 m**, with and without nucleation on subgrain boundaries (s. g. b.). It can be seen that providing an additional set of nucleation sites accelerates the $M_{23}C_6$ precipitation kinetics, increases slightly the number of $M_{23}C_6$ precipitates, and has some effect on the maximum value of mean radius attained by cementite precipitates before they redissolve.
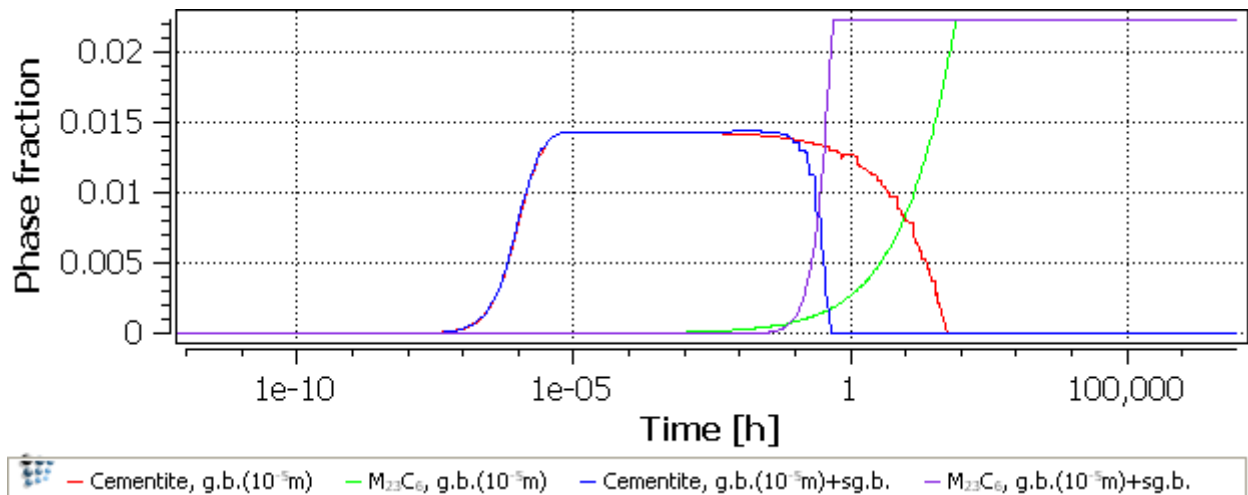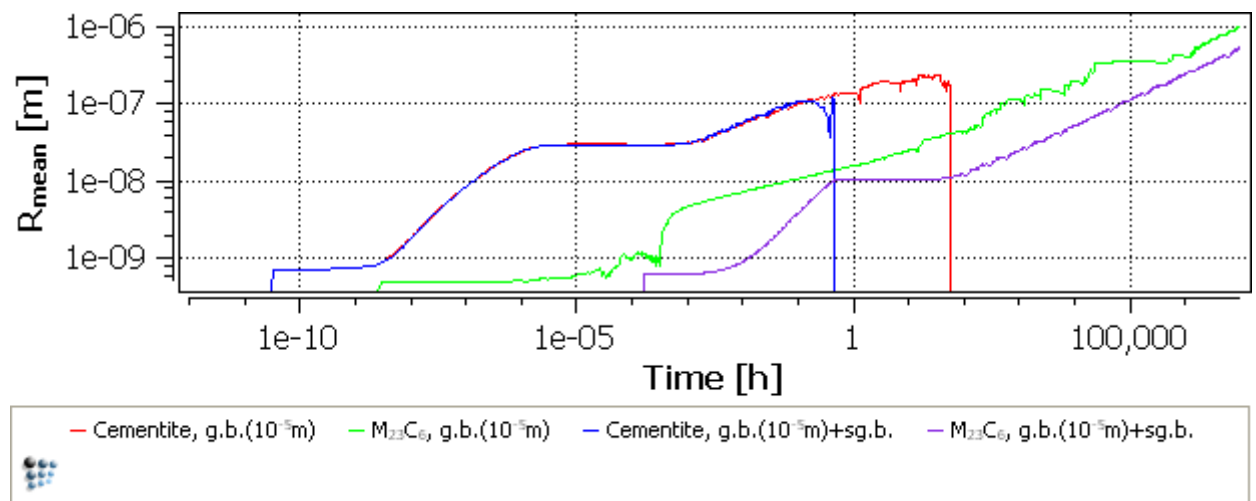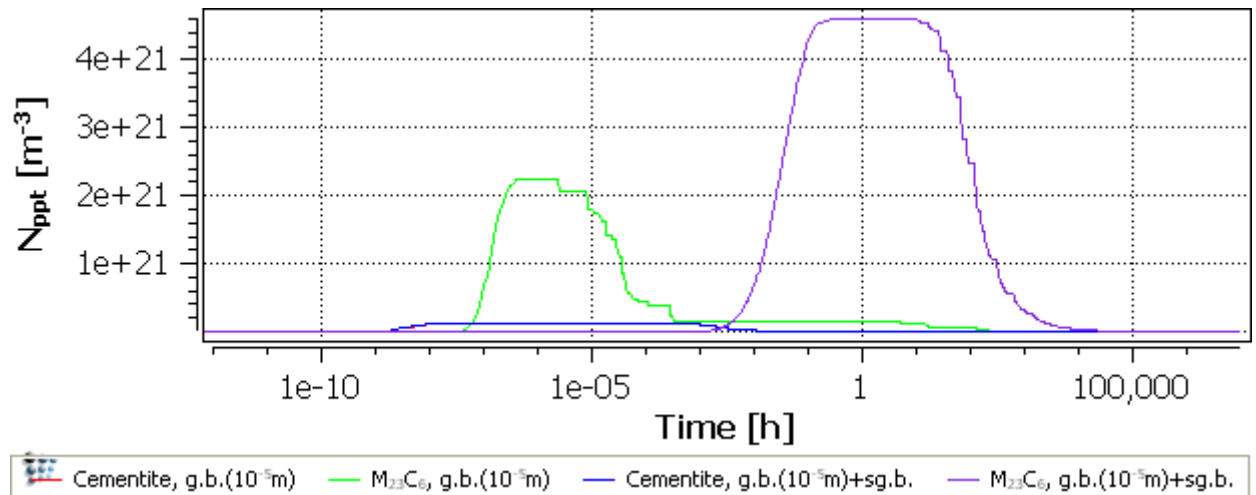
Elongated subgrains, obtained by increasing the subgrain elongation factor to 10, have a very small effect on precipitation and coarsening rates but influence the number of precipitates.
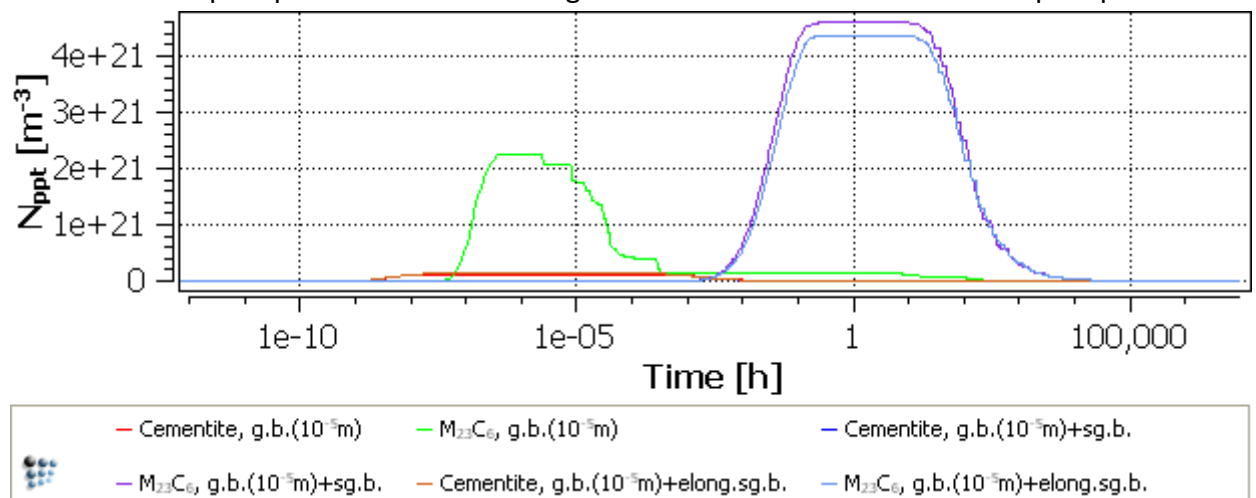
CONSECUTIVE ARTICLES

The tutorial is continued in article T17 - Multi-stage heat treatment

T17: COMPLEX MULTI-STAGE HEAT TREATMENTS

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb; ; mc_sample_fe.ddb

In this tutorial, we simulate the precipitation of NbC in the solid state during the continuous casting of steel and the subsequent austenitization treatment. The austenite / ferrite transformations of the matrix phases are taken into account. The continuous casting simulation starts at 1400°C with linear cooling to room temperature. The austenitization treatment is carried out at 1100°C for 2 hours. Heating and cooling rates are assumed to be 1 K/s. Furthermore, we assume that precipitation of NbC occurs only at austenite grain boundaries in the austenite during continuous casting. After transformation to ferrite, we assume that precipitation occurs at grain boundaries and dislocations.

CONTENTS:

- Definition of complex heat treatments
- The heat treatment editor
- Multiple precipitation domains / matrix phase transformations

SETTING UP GUI, THERMODYNAMICS, PRECIPITATES AND PRECIPITATION DOMAINS

SETUP CALCULATION

Create a workspace with the elements Fe, Nb and C and the phases BCC_A2 and FCC_A1. Enter the composition 0.1 wt.% C, 0.7 wt.% Nb. Create a precipitation domain named **'austenite'** with the phase FCC_A1 as its matrix, and a precipitation domain named **'ferrite'** with the phase BCC_A2 as its matrix. Create a precipitate phase FCC_A1#01_P0. Enter 25 as the number of size classes for this phase, and attach it to the **'austenite'** domain. The phase status dialog should look somehow like the figure below. Leave all the other settings at their default values. Read in the mobility data.
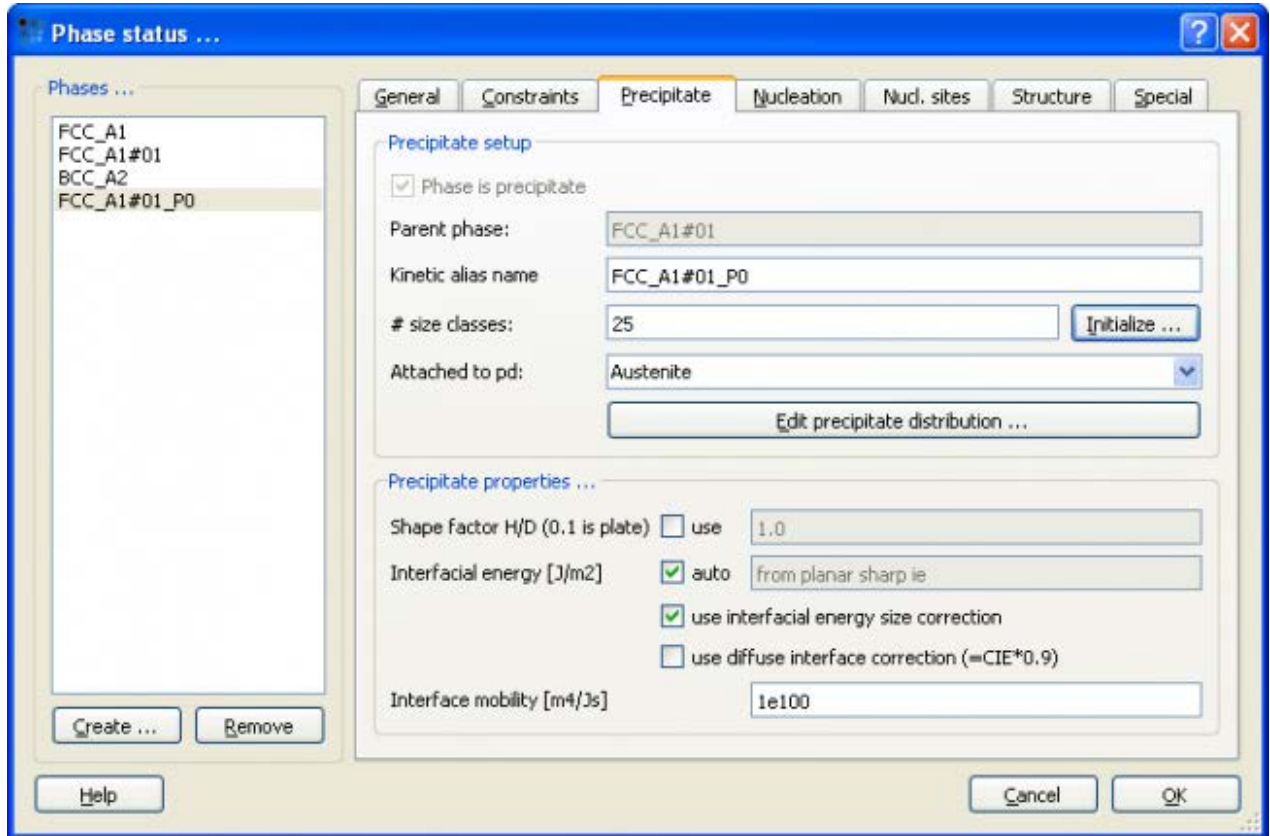
Setup GUI

Create a new XY-plot window with four plots in it. Use a default x-axis and set the axis type to 'log'. Scale from '10..'. The axis title is 'time / s'. Insert series into the plots as follows:

1. **T$C** (temperature in celsius), y-axis title **'Temperature [°C]'**.
2. **F$FCC_A1#01_P0** (phase fraction of NbC), y-axis title **'NbC phase fraction'**.
3. **R_MEAN$FCC_A1#01_P0** (mean radius of NbC), y-axis title **'mean radius [nm]'**, scaling **'0.1..'** and **'log'** type. Factor is **'1e9'** to display the radius in nm instead of m.
4. **NUM_PREC$FCC_A1#01_p0** (number density of NbC), y-axis title **'number density [m⁻³]'**. axis has **'log'** type and the scaling is set **'1..'**.

DEFINITION OF THE HEAT TREATMENT

Open **'Global → Heat treatments …'**. This dialog represents a very useful editor for definition of complex heat treatments by a sequence of linear heat treatment segments.
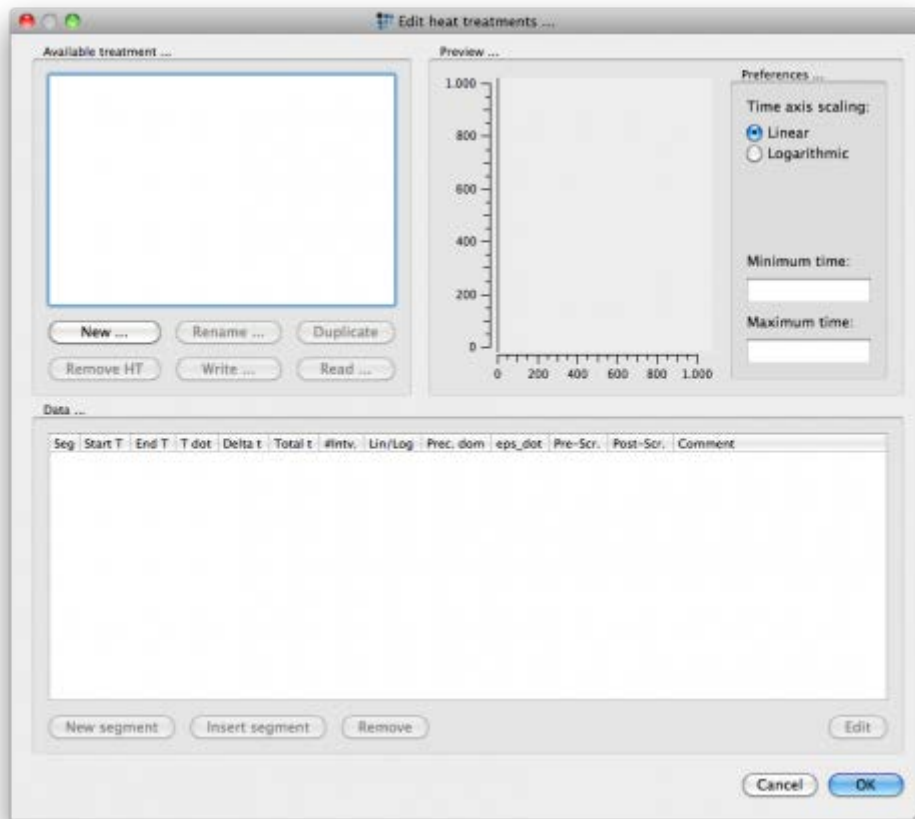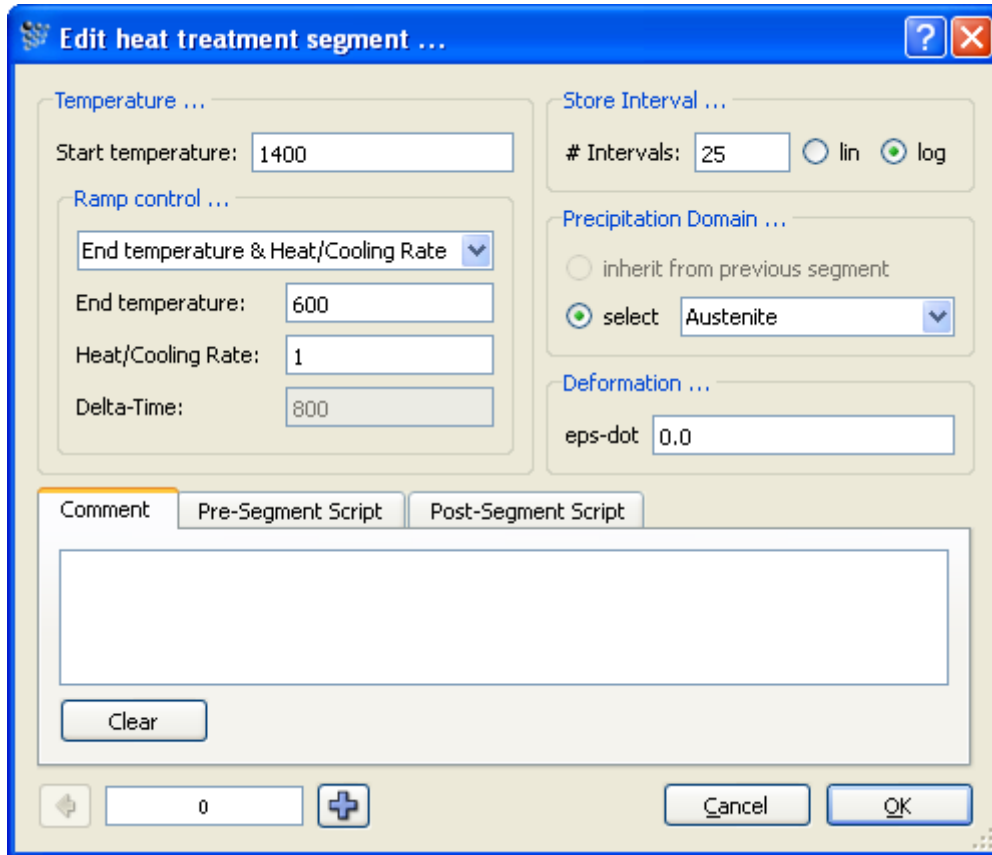
Firstly, create a new heat treatment **'New …'** with the name **'sample_ht'**.

Since the present steel will transform from austenite to ferrite during the cooling process, we start with setting up a linear cooling segment from 1400°C to transformation temperature with a cooling rate of 1 K/s. Let us assume that this transformation occurs instantaneously at 600°C. Create a new segment with the button **'New segment'**. Double-click the new line in the **'Data…'** list box or highlight the line and press **'Edit'**. In the following dialog, you can define the properties of the heat treatment segment. First of all, enter **'Start temperature'** 1400°C. Then, in the temperature definition mode combo box, you can select which data you want to provide to define the segment. Since we want to cool to RT and know the cooling rate, we select **'End temperature & Heat/Cooling rate'**. **'End temperature'** is 600°C and **'Cooling rate'** is -1.

The next important setting is the definition of the number of states to store during the calculation. By default, each segment stores 25 states with linear interval distances. Optionally, you can select logarithmic. Remain with the default settings.

Finally, select the precipitation domain for the segment, in our case **'austenite'**. The dialog should now appear like this:

To set up the next segment, press the ⊞ button. Choose **'Yes'** in the dialog asking about the creation of a new segment. The start temperature for each following segment is automatically set to the end temperature of the previous segment, that is 600°C. Enter the new end temperature (25°C) and select ferrite for the precipitation domain.

The second segment should look like this:
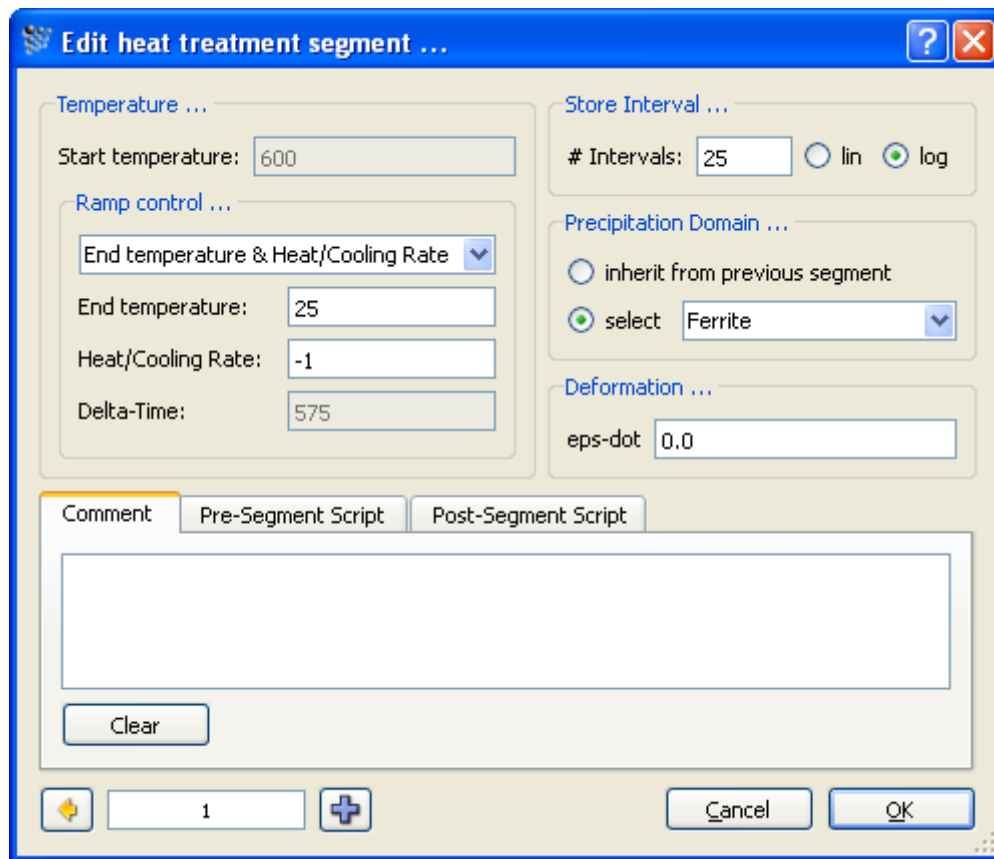
Continue to define the rest of the segments:

- Segment from RT to 850°C with 1 K/s heating rate. Since the precipitation domain does not change, select the **'inherit from previous segment'** radio button. We assume that the ferrite to austenite transformation occurs at 850°C.

1. Next segment from 850°C to 1100°C, however, with austenite as the precipitation domain (heating rate 1 K/s).
2. an isothermal segment for two hours at 1100 °C. This time, the temperature definition mode is **'End temperature & Delta-Time'**. End temperature is 1100°C and **'Delta-time'** is 7200 s (you can enter 2*60*60 as well).
3. Define a cooling segment down to 600°C in austenite matrix (cooling rate 1 K/s).
4. Finish with a segment from 600°C to RT having ferrite as a matrix (cooling rate 1 K/s).

If you have finished entering the segments, the entire heat treatment should look like this:
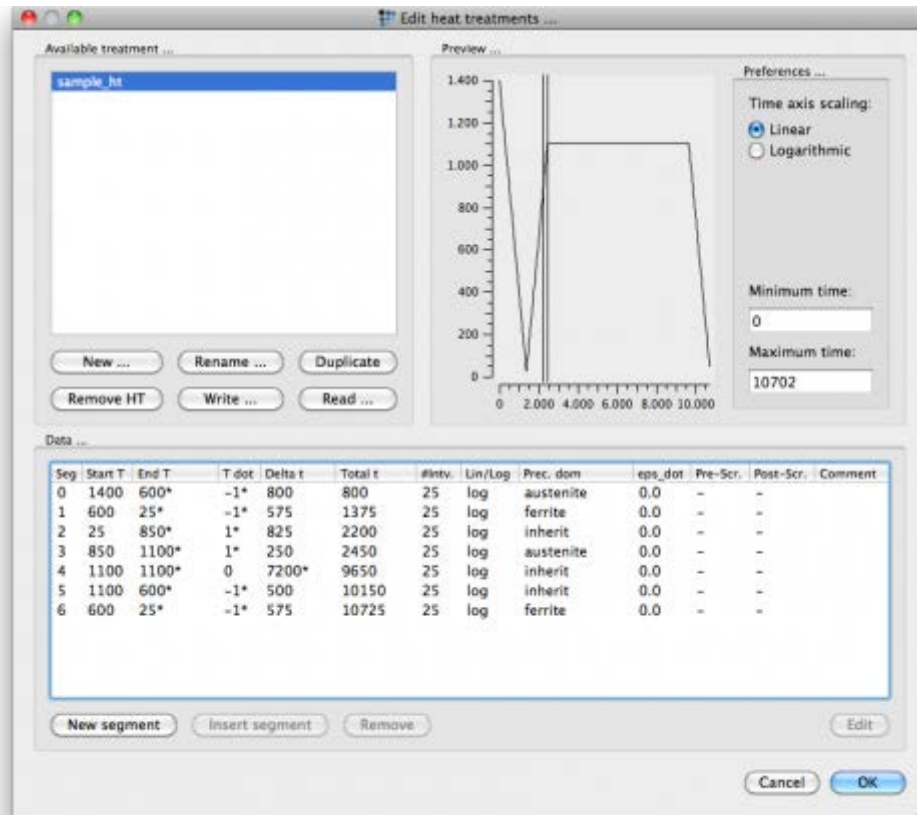
The last thing that we have to take care of is the changing nucleation sites for the NbC precipitates. According to our problem, we want to simulate NbC precipitation during cooling from continuous casting along the austenite grain boundaries. For all other parts of the heat treatment, we want to allow precipitation at grain boundaries and dislocations simultaneously.

This issue can be solved easily with the use of scripting commands that can be entered at the beginning and end of each of the heat treatment segments. Edit the first segment by double clicking it in the list. In the edit field for the pre-segment script, enter the command just as if you would do in the MatCalc console:

```
set-precipitation-parameter fcc_a1#01_p0 N S G
```

This command defines the (n)ucleation (s)ites of the NbC to be at (g)rain boundaries. Since only grain boundaries are selected, please note that MatCalc will then use the diffusion geometry for grain boundary precipitates, which has been introduced MatCalc version 5.14. The following images show the two different diffusion geometries of MatCalc:
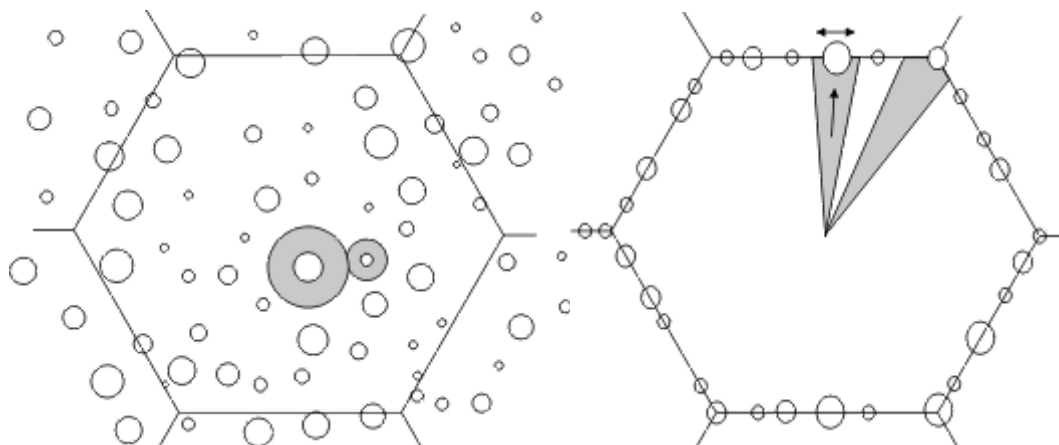
Since we want to continue with different nucleation sites after the first cooling segment, we define a post-segment script for the first segment reading

```
set-precipitation-parameter fcc_a1#01_p0 N S DG
```

This command will define (d)islocations AND (g)rain boundaries as nucleation sites. MatCalc will then automatically use the spherical diffusion geometry again as shown in the left image.
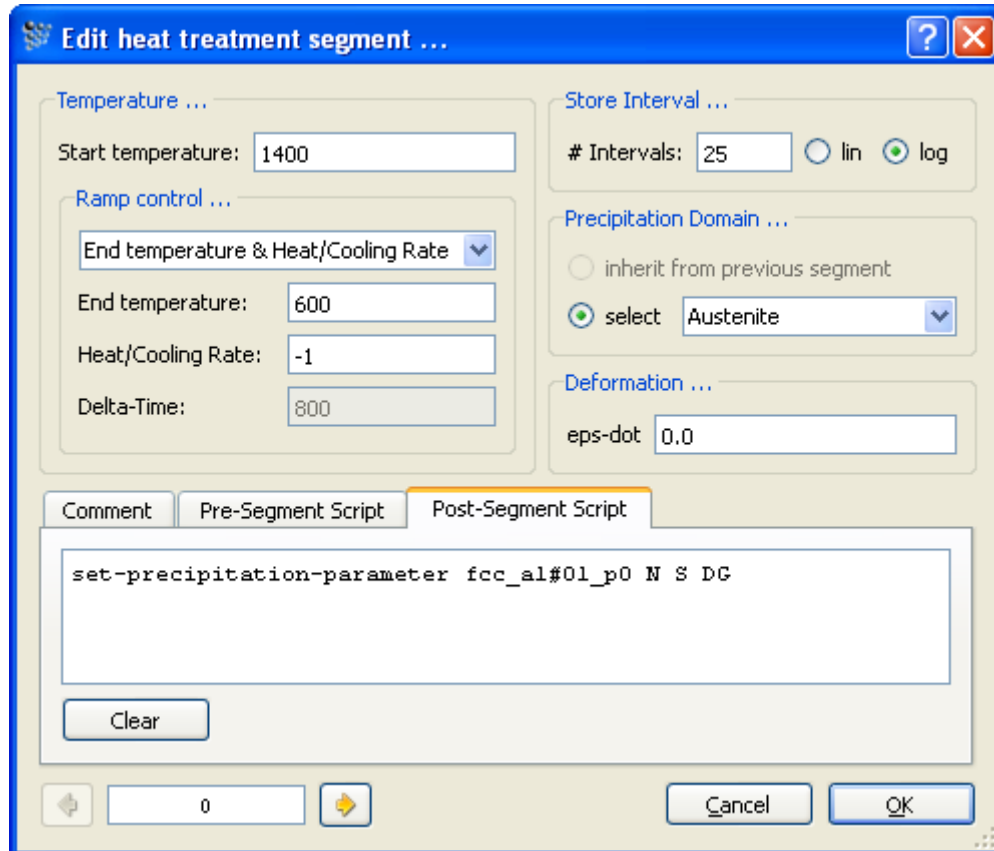
Click **'Ok'** to go the heat treatment editor. The existence of pre-segment and post-segment scripts is indicated by the letter **'Y'** in the heat treatment editor.

Again, click **'Ok'** and **Save** your file (**'tut17.mcw'**).

PERFORM SIMULATION

Start the precipitation simulation with **'Calc → Precipitate kinetics …'**. In this dialog, the most important setting is the **'temperature control'** selection. Select **'from heat treatment'** and **'sample_ht'**. It is not necessary to enter/modify the simulation end time because MatCalc will automatically stop when reaching the end of the heat treatment segments.
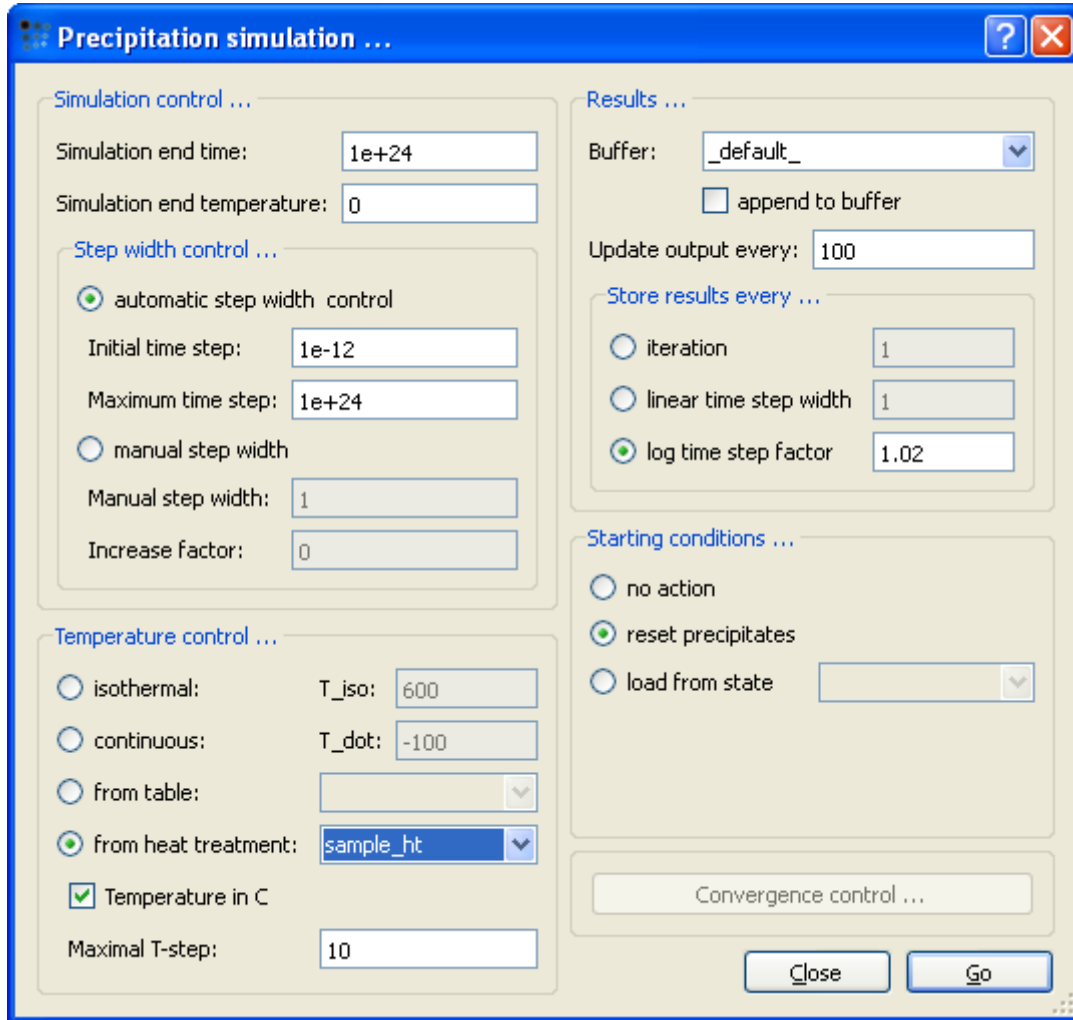
Start the precipitation simulation with the **'Go'** button.

After reaching the end of the heat treatment, the results look like follows:
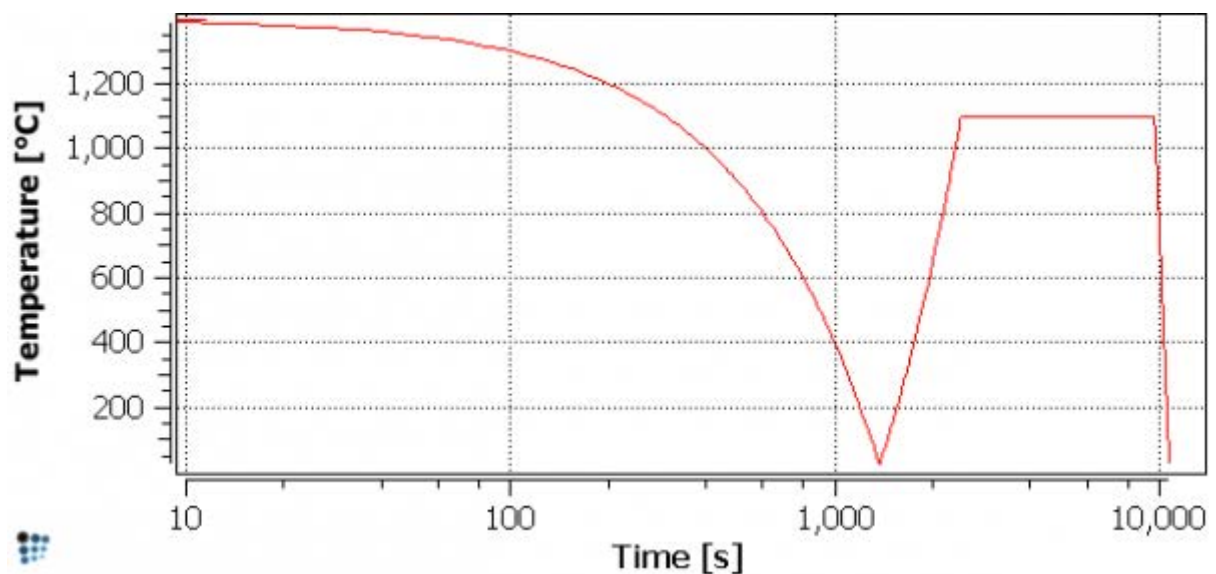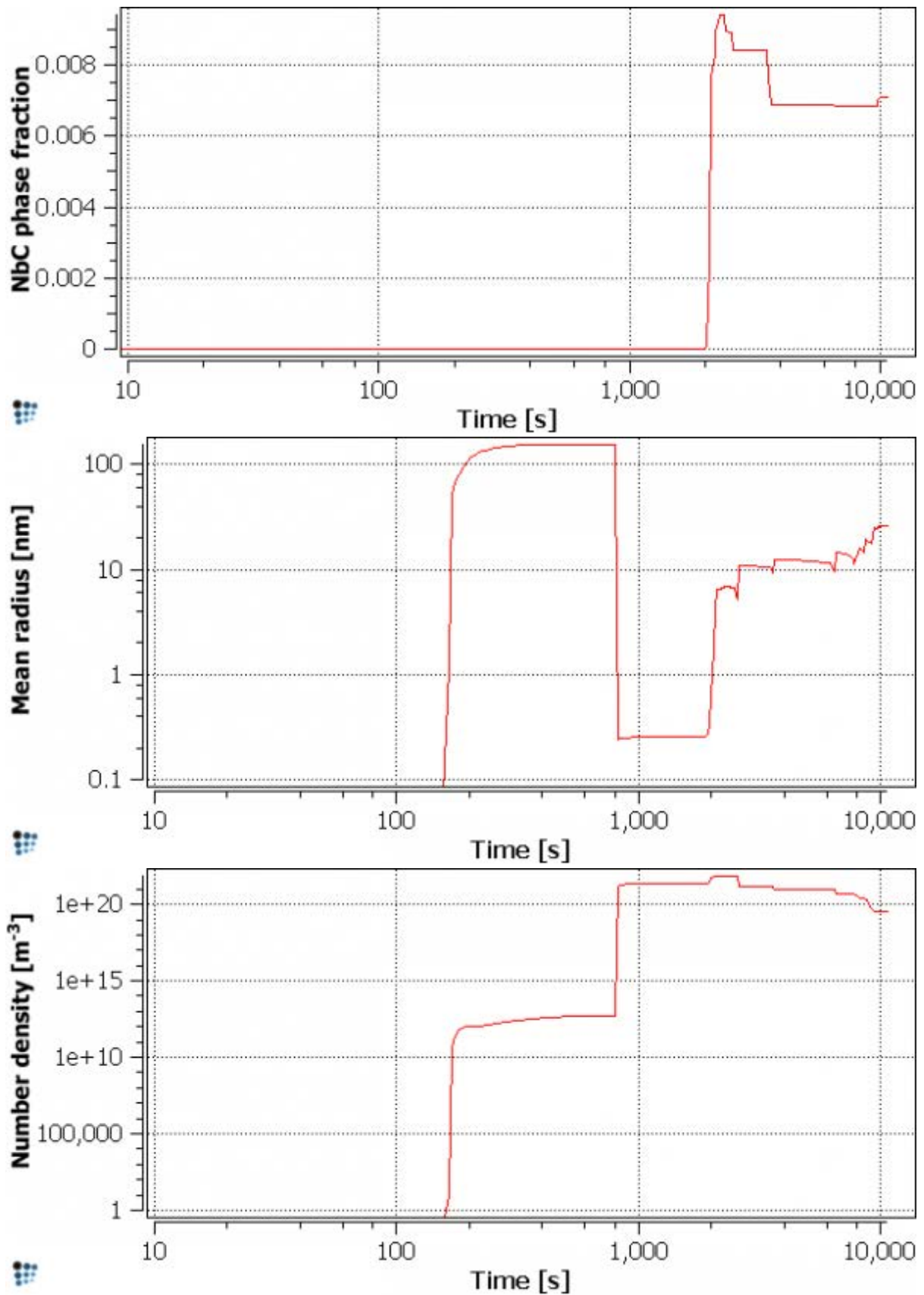
The temperature plot on top shows the expected profile. The next plot with the NbC phase fraction shows a strong increase of the phase fraction at around 2000s, where the specimen reaches about 800°C on heating. Later, during austenitization, the phase fraction is decreased

slightly because the solubility of the Nb and C is increased. The phase fraction remains almost constant during the rest of the process.

When looking at the plots for the mean radius and the number density of the NbC precipitates, interpretation of the results is more difficult. First, nucleation starts and proceeds until 200 s. The nucleation stops because there are no more available nucleation sites at the grain boundary. Up to approximately 800 s, the existing NbC precipitates only grow. After switching to ferrite and adding dislocations as additional nucleation sites, the number density quickly increases in a burst of nucleation events. At the same time, the **mean radius** drops drastically, which is at first sight unexpected. However, since the plot displays the mean radius of the precipitate population, generation of a large number of new and small precipitates will decrease the mean value to the value of the highest number of precipitates. Later, in two more steps, the radius increases again due to growth as well as dissolution of a part of the small precipitates generated in the second nucleation burst.

Apparently, interpretation of this kind of simulation suffers from the fact that two different kind of precipitate populations, namely the one on the austenite grain boundaries and the other on the dislocations are treated as one. In the following section, a method of separation of populations is used that can be very useful in complex simulations.

SIMULATION WITH SEPARATION OF PRECIPITATE POPULATIONS

On many occasions, it can be useful to separate populations of one and the same precipitate type to facilitate interpretation of the results. For the present example, this is easily done by introduction of an additional precipitate phase FCC_A1#01_P1. Create an additional precipitate based on the FCC_A1#01 parent phase in the **'phase status ….'** dialog. Highlight the FCC_A1#01 phase and press **'Create …'** for a new precipitate phase.Go to the 'Precipitate' tab and initalize the new phase with 25 classes.
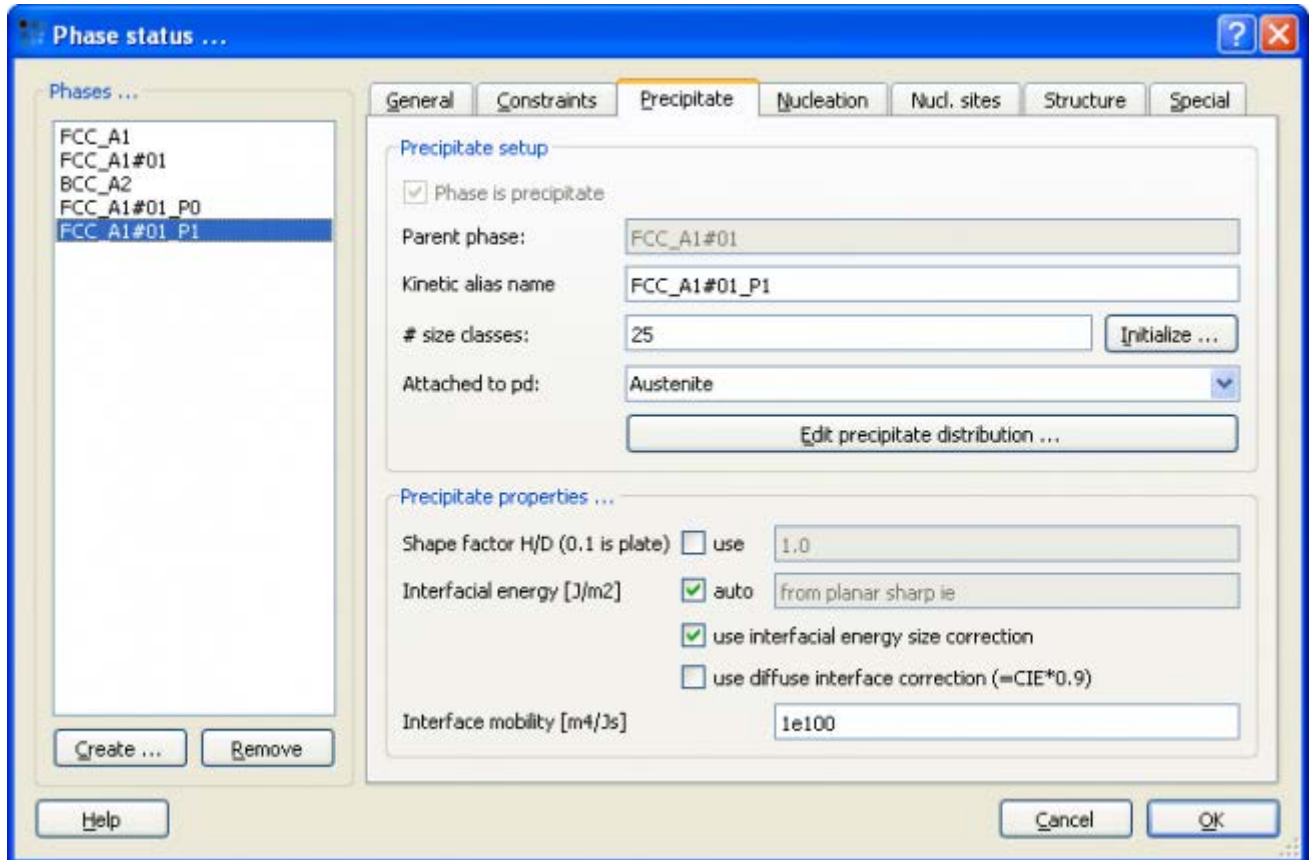
Note that the suffix **'_P1'** of the new phase indicates that the precipitate is identical to the **'_P0'** in terms of its nucleus composition, however, it contains precipitate classes that can have appeared at different stages of the heat treatment.

Let us now set up the simulation such that the _P0 phase can only nucleate in the first segment of the heat treatment, that is cooling in the austenite, while the **'_P1'** population is not allowed to form. This can be done by defining **'nucleation sites' as 'none'**. For all consecutive segments, nucleation of further **'_P0'** precipitates will be suppressed while the **'_P1'** population can nucleate at grain boundaries and dislocations.

Make the following changes to the pre-segment and post-segment scripts of the first segment in the heat treatment editor:

```
Pre-Segment    Post-Segment

SET-PRECIPITATION-PARAMETER FCC_A1#01_P0 N S G
SET-PRECIPITATION-PARAMETER FCC_A1#01_P1 N S N

    Clear
```

```
Pre-Segment    Post-Segment

SET-PRECIPITATION-PARAMETER FCC_A1#01_P0 N S N
SET-PRECIPITATION-PARAMETER FCC_A1#01_P1 N S DG

    Clear
```

Run the simulation again and modify the plots to display the properties of both precipitate populations. The result should look like this:
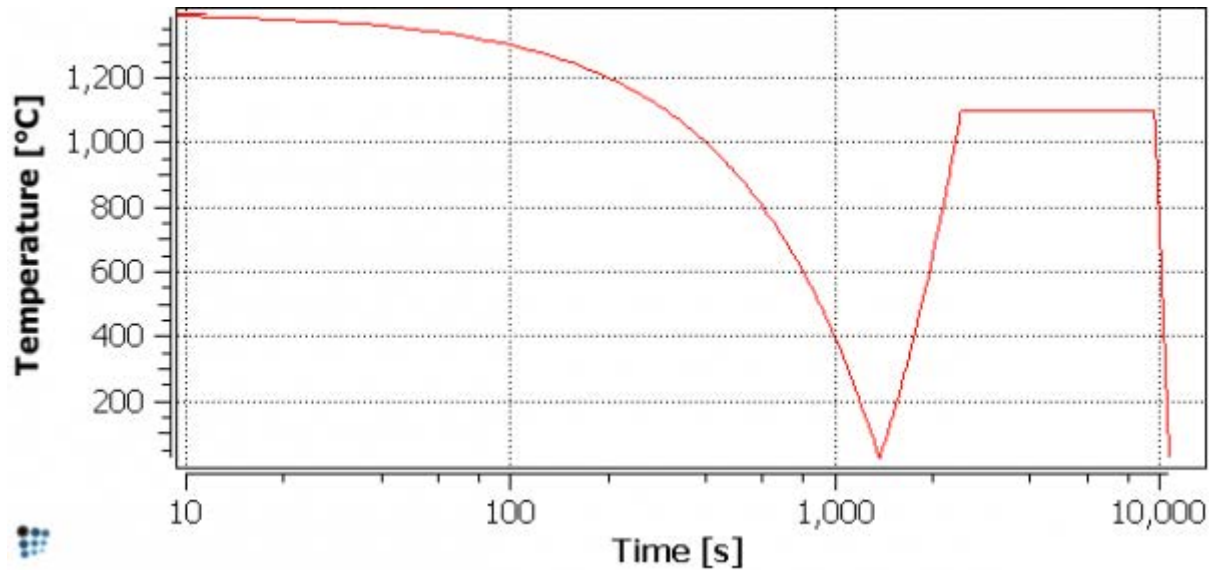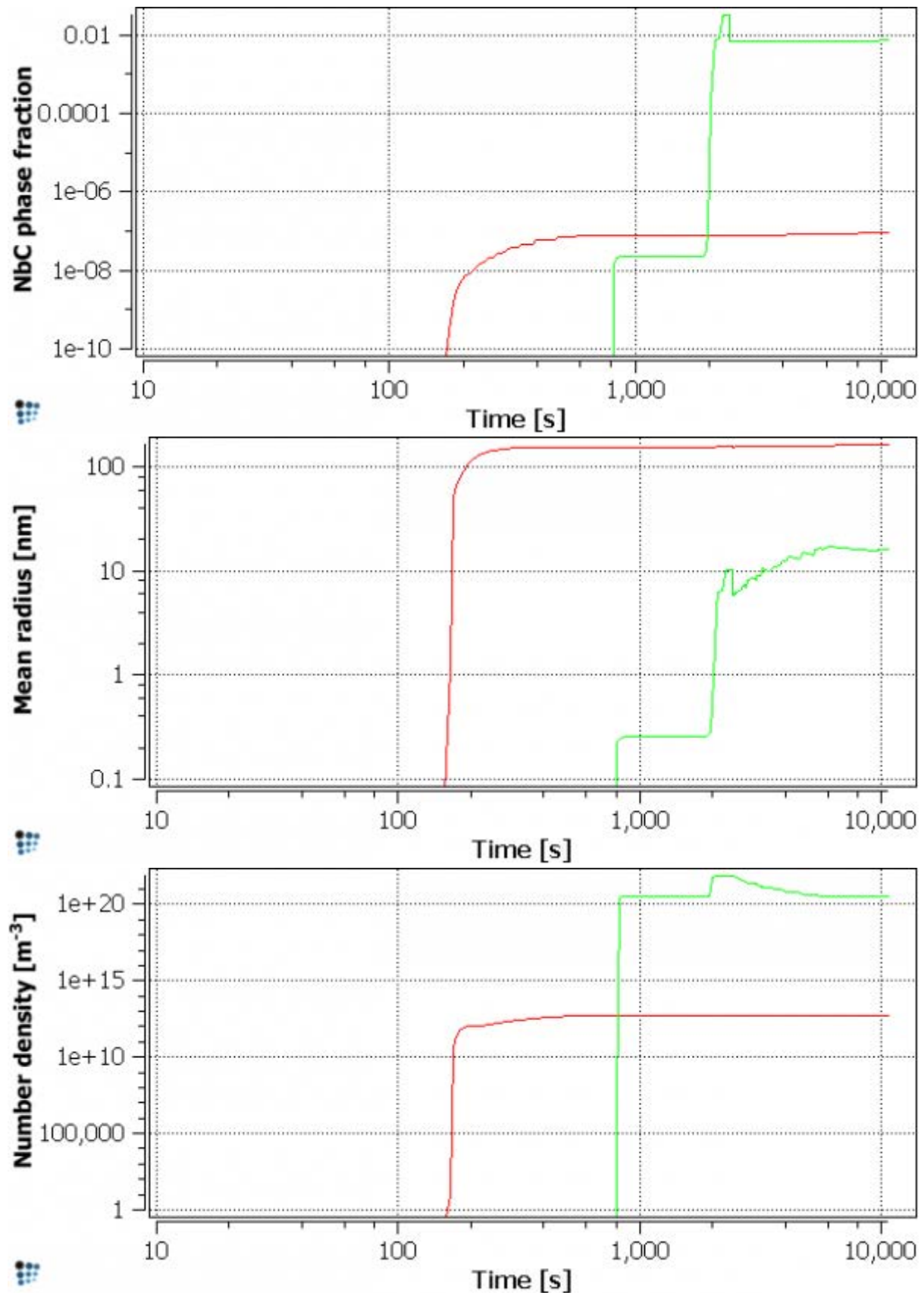
Major advantage of simulations with separated precipitate populations is the ease of interpretation of the results. The second simulation clearly shows that the precipitates that are formed during cooling in the austenite grow to large size and remain almost unaltered

during the later stages of the heat treatment. On the other hand, their phase fraction and number density is low, which indicates that their contribution to mechanical properties in terms of precipitation strengthening will be negligible. The second population appears in high number density and with small radius of approximately 10 nm. Moreover, the phase fraction is high, indicating a strong potential for precipitation strengthening of this second wave of NbC precipitates.

CONSECUTIVE ARTICLES

The tutorial is continued in article T18 - TTP (time-temperature-precipitation) diagrams

T18: PLOTTING A TTP DIAGRAM

This tutorial was tested on
MatCalc version 5.50 rel 0.057
license: free
database: mc_sample_fe.tdb; ; mc_sample_fe.ddb

CONTENTS:

- Calculating a TTP diagram for isothermal treatments
- Calculating a TTP diagram for continuous cooling
- Plotting the diagram
- Display options: absolute, relative or relative to maximum phase fraction

A time-temperature-precipitation diagram is a plot consisting of contours characterising the extent of a precipitation reaction on axes of temperature versus time. In this tutorial, a TTP diagram will be calculated for the precipitation of NbC in the austenite single-phase region.

SETTING UP THE SYSTEM

Create a workspace with the elements Fe, Nb and C and the phases BCC_A2 and FCC_A1. Enter the composition 0.1 wt.% C, 0.7 wt.% Nb. Firstly, it is necessary to determine the extent of the austenite single-phase region in which the TTP diagram is to be calculated. To do this, first calculate an equilibrium at 1000°C and then search for the BCC_A2 phase boundary (referring to Tutorial 7 if necessary). This gives a temperature of 903.51°C for the zero-phase-fraction boundary of BCC_A2. This is the upper boundary of the low-temperature **'alpha'** form of ferrite. Next, calculate another equilibrium at 1200°C and repeat the procedure. This time, the temperature value found is 1439.01°C, which is the lower boundary of the high-temperature **'delta'**-ferrite. Between these two limits, the only stable matrix phase is austenite (FCC_A1). Perform a stepped equilibrium calculation between 920°C and 1430°C with 10°C step and plot the phase fraction of FCC_A1#01 phase depending on the temperature.

Create a precipitation domain named **'austenite'** with the phase FCC_A1 as its matrix, and a precipitate phase FCC_A1#01_P0. Enter **'25'** as the number of size classes for this phase, and attach it to the **'austenite'** domain. Its precipitation sites should be dislocations. Leave all the other settings at their default values. Read in the mobility data.

TTP DIAGRAMS FOR ISOTHERMAL HEAT TREATMENTS

CALCULATIONS OF PHASE FRACTION FOR ISOTHERMAL TREATMENTS

The plot below, obtained using a stepped equilibrium calculation, shows the equilibrium phase fraction of NbC between 925 and 1425°C:
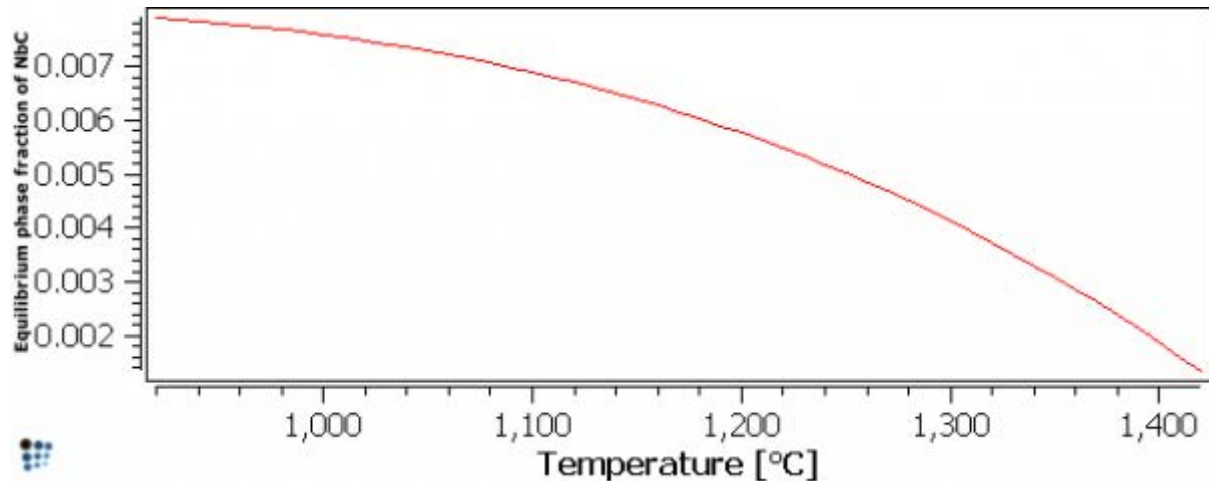
The plot below illustrates the origin of the typical C-shaped curves of TTP plots. It was obtained using **'Calc > Precipitation kinetics'** to simulate an isothermal heat treatment at 925°C, plotting the series **F\$FCC_A1#01_P0** on a logarithmic x-axis, then duplicating and locking this series before making further calculations in the same way at a selection of other temperatures. At each value of temperature, the phase fraction of NbC increases with time before reaching a plateau when the equilibrium phase fraction of NbC at that temperature is attained. It can be seen that, between 1025 and 1125°C, the rate of reaction first increases (characterised by a shift of the curve towards the left), goes through a maximum, then decreases again. TTP diagrams plot the time taken to reach a particular point in a reaction at different temperature values. It can be seen from the plot below that if, for example, the time taken to reach 90% of the plateau value were plotted for each temperature on axes of temperature versus time, the resulting curve would be C-shaped. The TTP diagram calculation function of MatCalc allows automatic calculation of curves of this type.
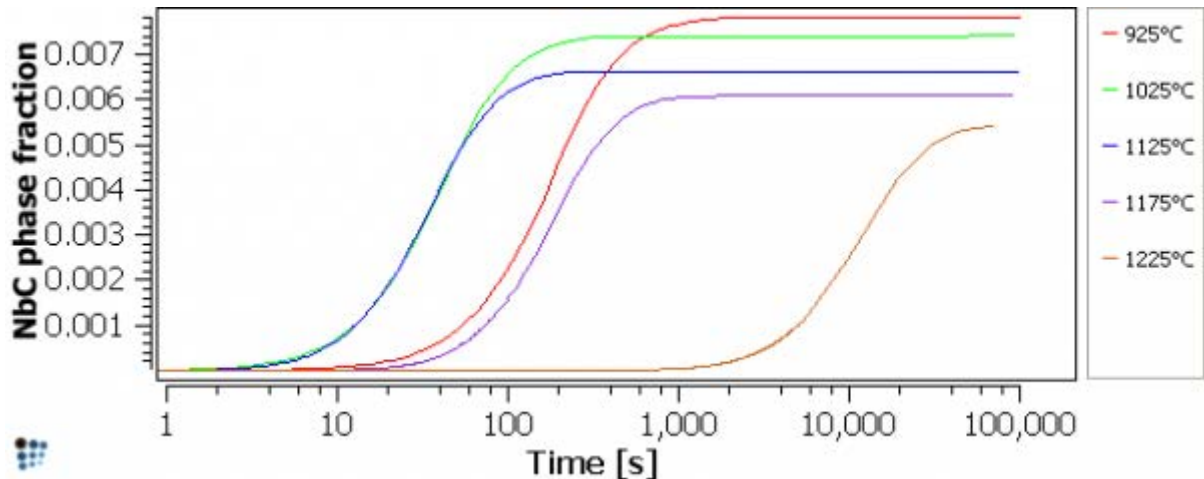
AUTOMATIC CALCULATION OF TTP DIAGRAMS

Open **'Calc > TTP-diagram'** and enter **'1425'** as the start temperature and **'925'** as the stop temperature. The end time should be sufficient for the phase fraction to reach a plateau at all temperatures under consideration. (This can be verified by creating an XY-plot of F$FCC_A1#01_P0 versus time and monitoring this during the TTP diagram calculation.)

In the **'Calculation method'** area, select **'isothermal'** and enter a value of 25 for **'delta T'**. Calculations will now be performed every 25 degrees between 1425 and 925°C.

Note: The calculation in the whole range may take more than 30 minutes (depending on your PC capacity). In case you would not spend so much time on this tutorial constrain the temperature range (e.g. 925°C - 1225°C)
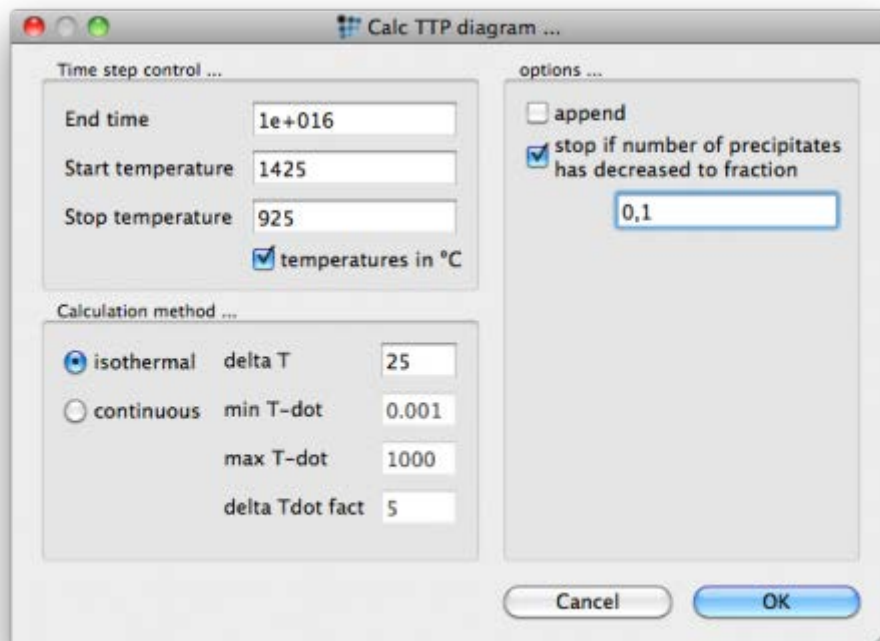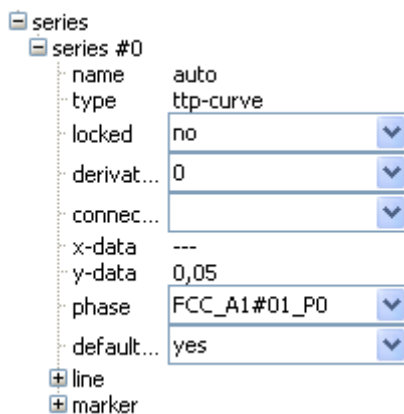
PLOTTING THE RESULTS

When the calculation has finished, create a new window of type **'(p6) Plot: TTP-diagram'**. In the **'options'** window, expand the **'plots'** section and right-click in the area under **'plot#0'** to show the context menu. Select **'new series'** and choose **'ttp-curve'** from the sub-menu on the right. Next, it is necessary to decide on the type of TTP contours required. The three options are:

- Absolute: the contours correspond to different values of the phase fraction F$FCC_A1#01_P0.
- Relative: a contour with a value of **'x'** for a particular temperature denotes the time at which the ratio of F$FCC_A1#01_P0 to its maximum value at that temperature is equal to **'x'**. The maximum values of F$FCC_A1#01_P0 are approximately equal to the equilibrium phase fractions F$FCC_A1#01 shown above.
- Relative max f: in this case, contour values represent ratios of F$FCC_A1#01_P0 to its maximum value overall. These contours have a similar form to the **'absolute'** contours, but different numerical values.

Select **'relative'** from the **'refer to f'** drop-box at the top of the **'options'** window. Then expand the **'series'** section of **'options'**, which should look as shown in the image below. Select the phase FCC_A1#01_P0 from the **'phase'** drop-box and enter **'0.05'** into the **'y-data'** line.

Add two more series to show the contours for ratios of 0.5 and 0.95 on the same diagram. The resulting diagram should look like this:
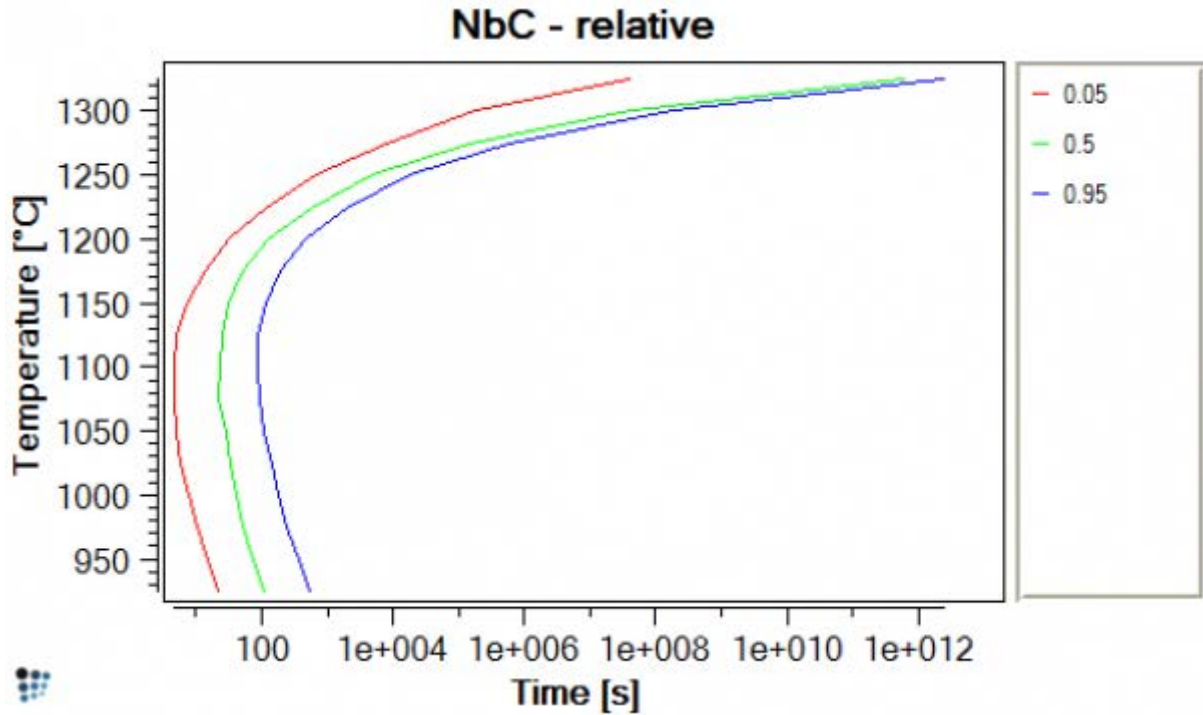
The following two plots are examples of the other types of TTP diagram. (TIP - to create more than one type of TTP diagram in the same plot window, lock all the series in the first diagram, then change the diagram type in the **'refer to f'** drop-box to plot the next diagram.)

ABSOLUTE

In the plot below, the contours correspond to different values of the phase fraction F\$FCC_A1#01_P0. Note that the higher values are only attained at lower temperatures, because the equilibrium value of F\$FCC_A1#01 decreases with increasing temperature. The maximum value of F\$FCC_A1#01_P0 is around 7.8e-3.
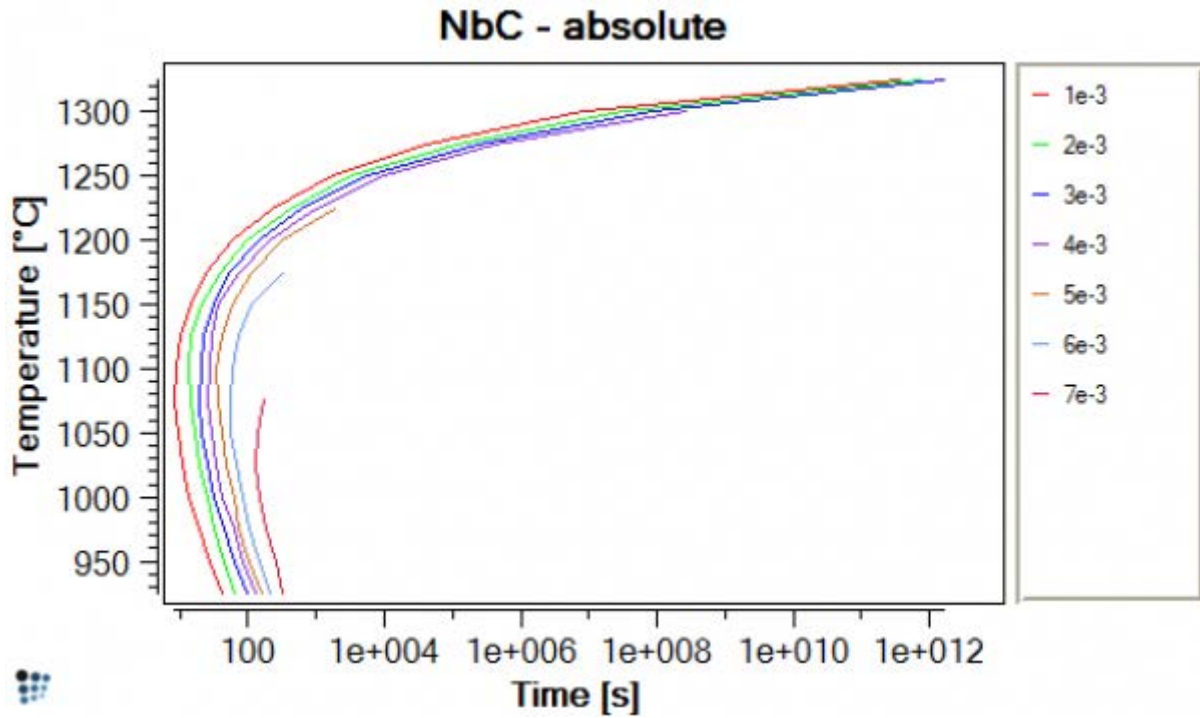

RELATIVE MAX F

This diagram has a similar appearance to the **'absolute'** diagram above, but the contours now represent different ratios of F\$FCC_A1#01_P0 to its maximum value.
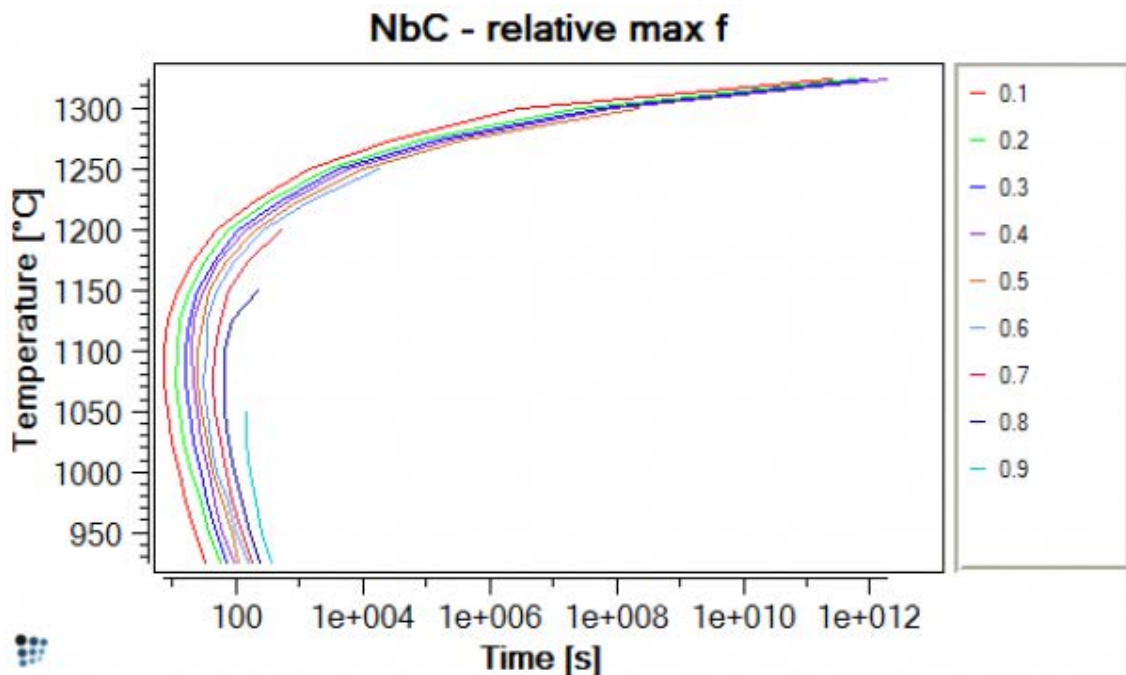
TTP DIAGRAMS FOR CONTINUOUS COOLING

TTP diagrams can also be calculated under conditions of a constant rate of temperature change. The diagram below shows several curves of phase fraction versus time for the temperature interval from 1425 to 925°C calculated with different cooling rates. It can be seen that the fraction precipitated is greater when cooling is slower, because the reaction has more time in which to occur.
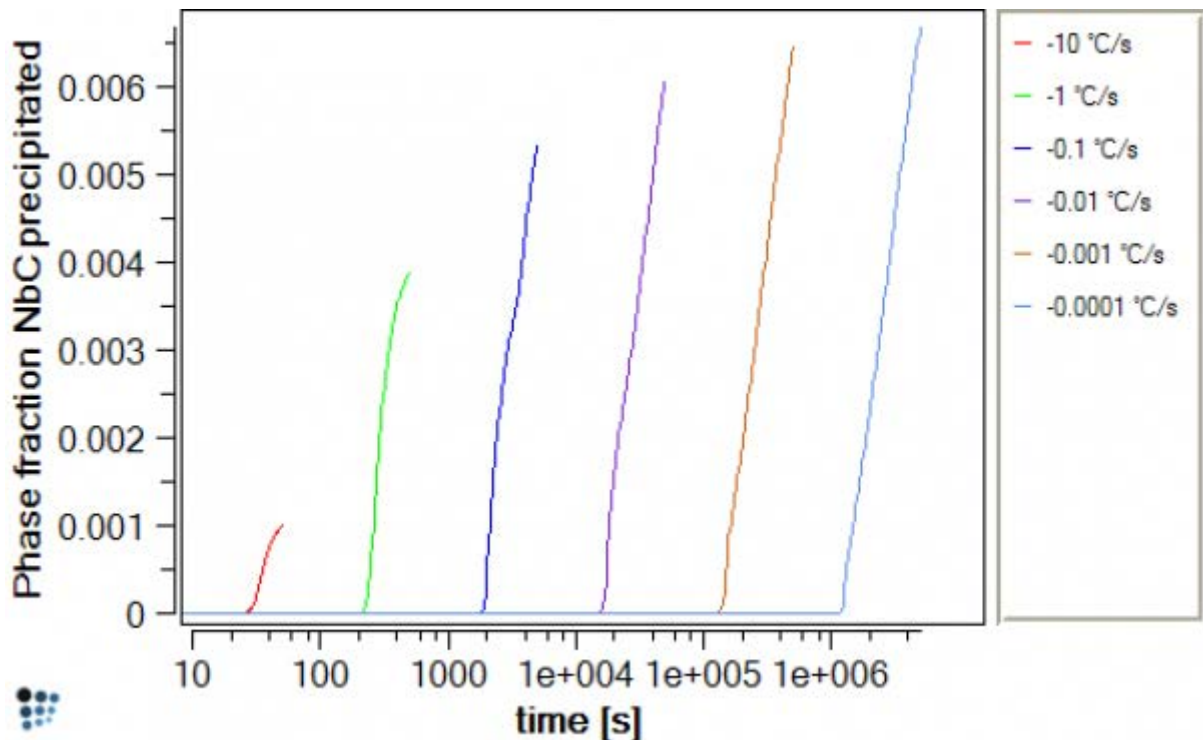
Continous-cooling TTP diagrams can be calculated as shown below. Enter a large value for the end time, otherwise this may cause the calculation to end before the stop-temperature is attained when slow cooling rates are used. Select **'continuous'** in the **'calculation method'** section and enter the **'0.0001'** and **'1000'** as the minimum and maximum cooling rates respectively, and **'5'** as the **'delta Tdot fact'**. Click **'OK'** to start the calculation.
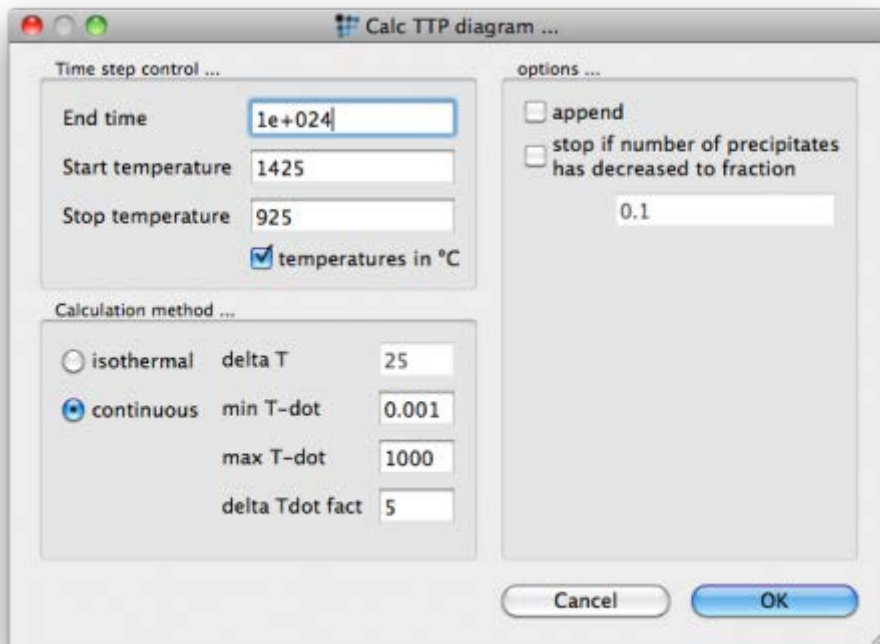
In the same way, the results can be displayed as absolute, relative or relative to the maximum phase fraction. The plot below shows contours of absolute values of phase fraction. In this case, logarithmic values have been used.
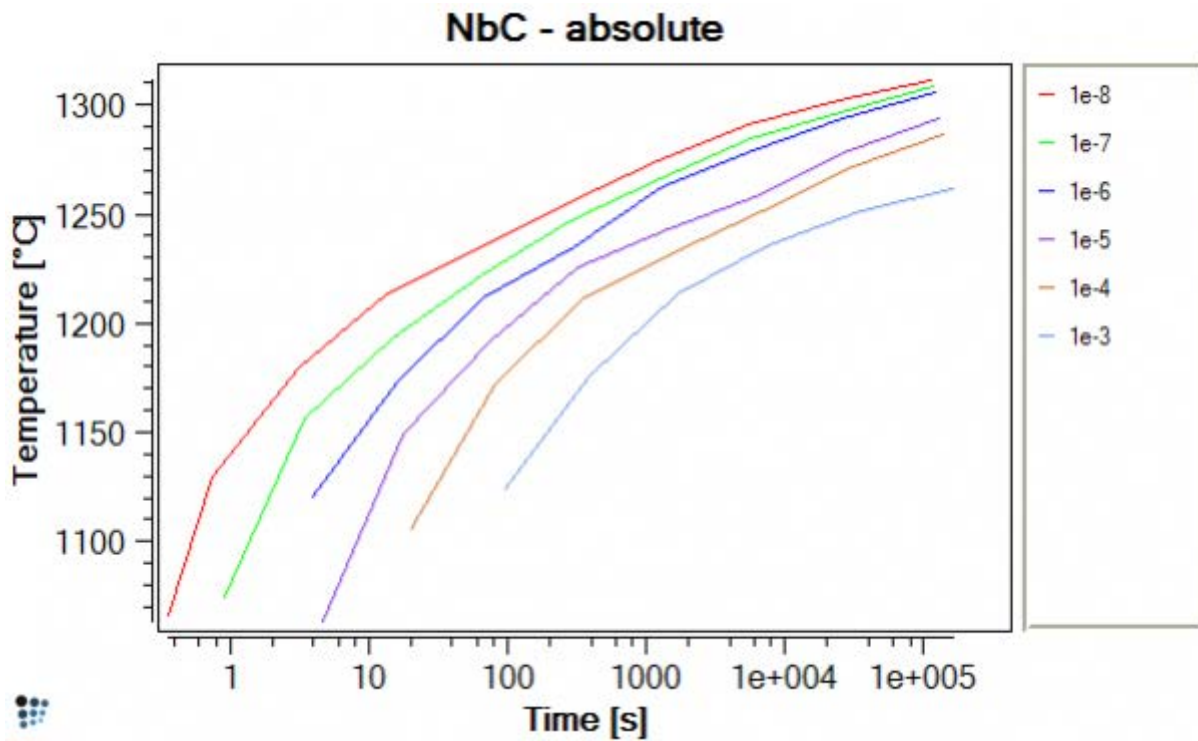
The image below is a **'relative'**-type plot, in which the contours represent the ratio of F$FCC_A1#01_P0 at a particular cooling rate to its maximum value attained at that cooling rate.