

MatCalc[®] User Manual

(Maintained by MatCalc Engineering)

This User Manual is aimed at demonstrating the basic handling of the MatCalc software. It starts with typical operations using the GUI, performing simple calculations of thermodynamic equilibrium and post-processing of the results in graphical form. If you are a new MatCalc user, try out the tutorial sections one by one. You will become acquainted to the basic features and functions of the software and learn how to set up your simulation problems.



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

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

database: none

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

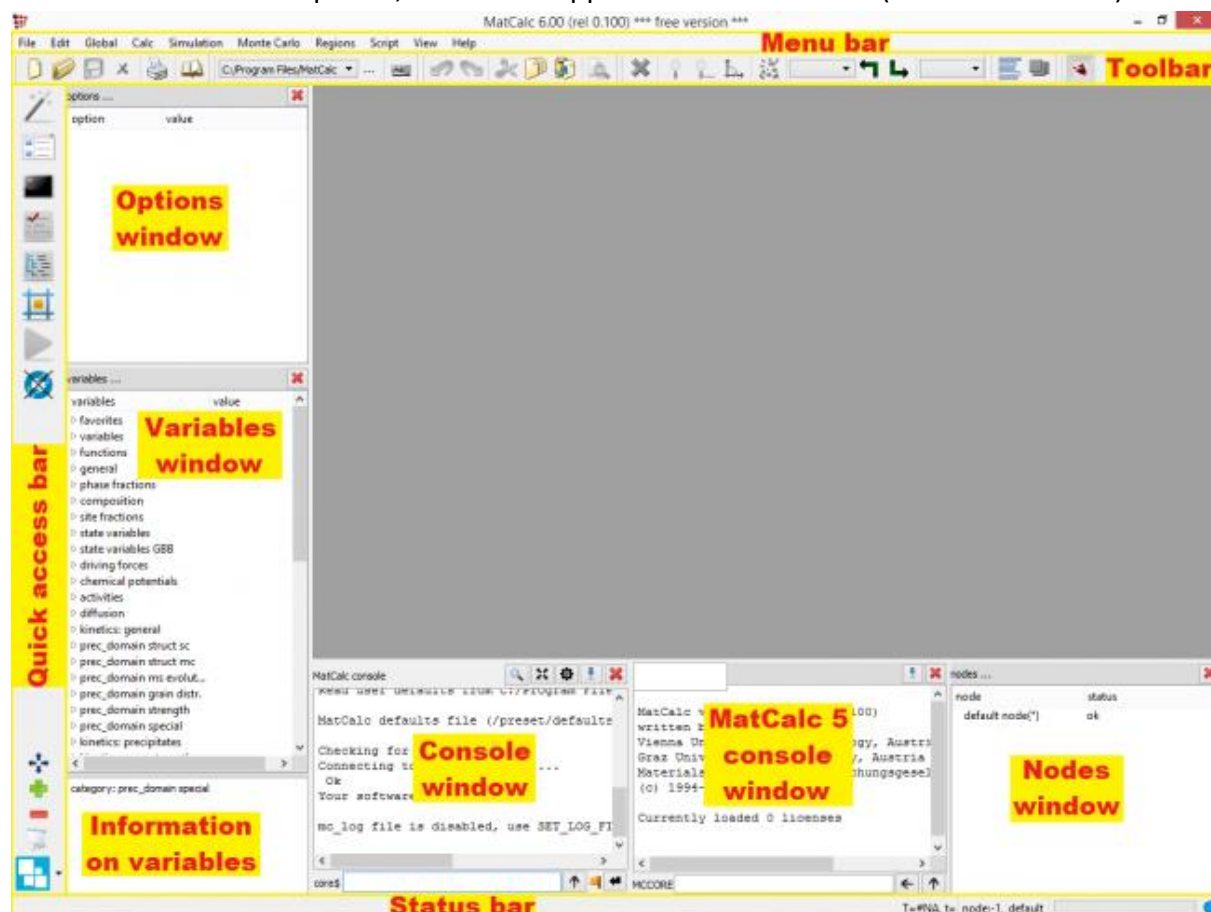
CONTENTS

- 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)

Quick access bar Icons giving quick access to window management options

Console Window for entering command-lines; more information is given below and in [Tutorial 12](#).

MatCalc 5 Console Window for entering command-lines, assuring compatibility with MatCalc 5 commands/scripts; 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.).

Nodes window List of nodes used in simulation. Multiple nodes are used in the advanced calculations

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', 'Regions': 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

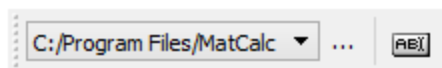
The toolbar area contains a number of icon groups:

'File etc'



L-R : New, open, save, close workspace, print, contents

'Dir'

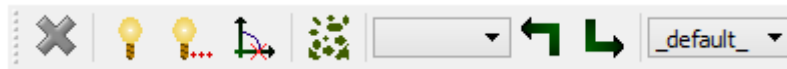


L-R: browse working directory, run script

'Edit'



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

'Calc'

L-R: Stop current action, single equilibrium, stepped equilibrium, search phase boundary, precipitate kinetics calculation, select calculation state, save into current calculation state, load from current calculation state, select calculation buffer.

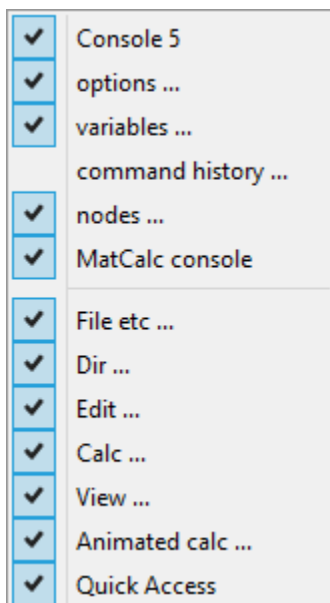
'View'


L-R: Show console, create new window.

'Quick access'

L-R: Wizard, hide all, console, options, variables, nodes, start, freeze all window updates, fit windows into viewport, zoom in, zoom out, open Navigator, Display Mode

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:

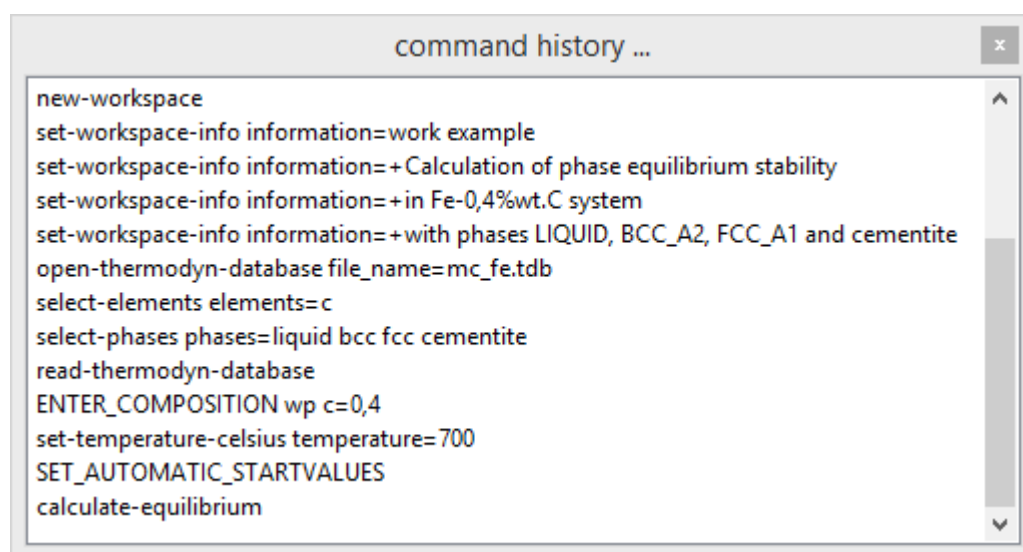
**CONSOLE**

This window allows command-line input, as an alternative to using the graphical controls. Commands can also be grouped into script files, for easier and more rapid execution of repetitive or complex tasks. More on the console, command-line syntax and scripts will be found in [Tutorial 12: Using the MatCalc console](#) and [Tutorial 13: Introduction to scripting](#). The console can be shown or hidden using **View > Show console**, pressing **F4** key or clicking on  icon.

MatCalc 6 uses a new formalism for the command-line input. While the scripts and commands used in the older versions are recognized by the current version, the old command formalism is to be typed in '**MatCalc 5 console**' window.

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.

Execute_and_Close	Enter
Copy + Close	Ins
Remove	Del
Remove all	
Close	Esc

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.

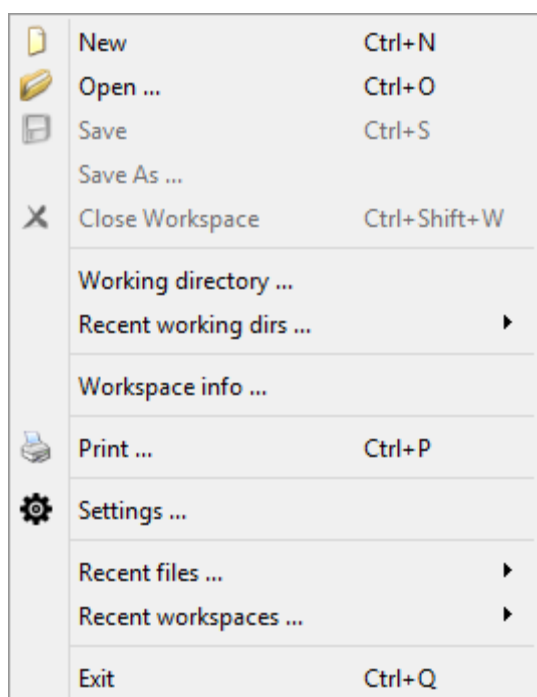
CONFIGURING THE LAYOUT

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

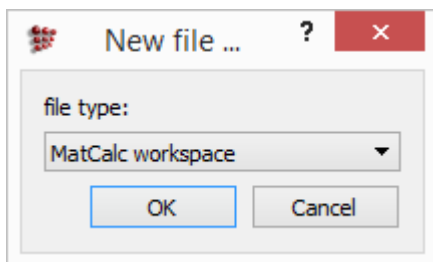
THE 'FILE' MENU

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

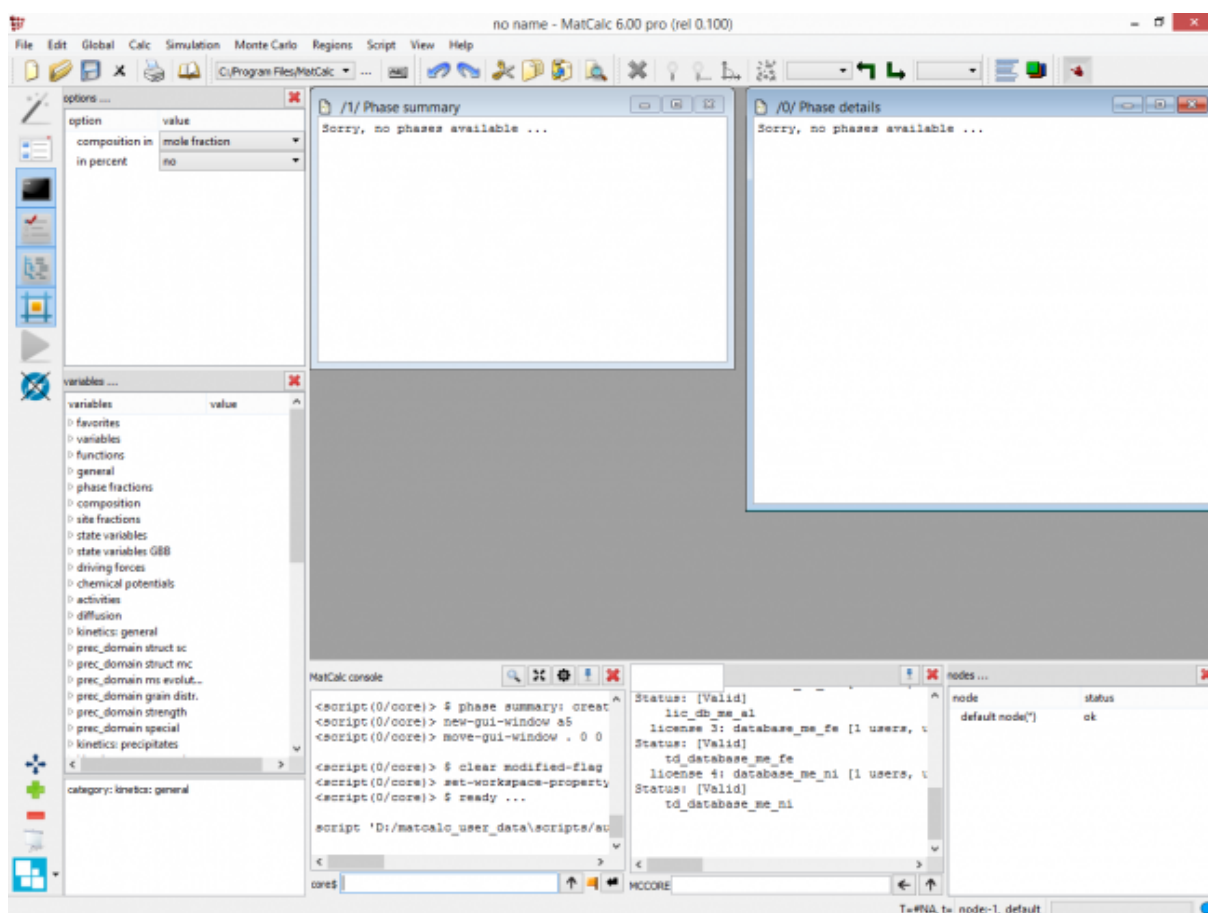


CREATING A NEW WORKSPACE FILE

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:

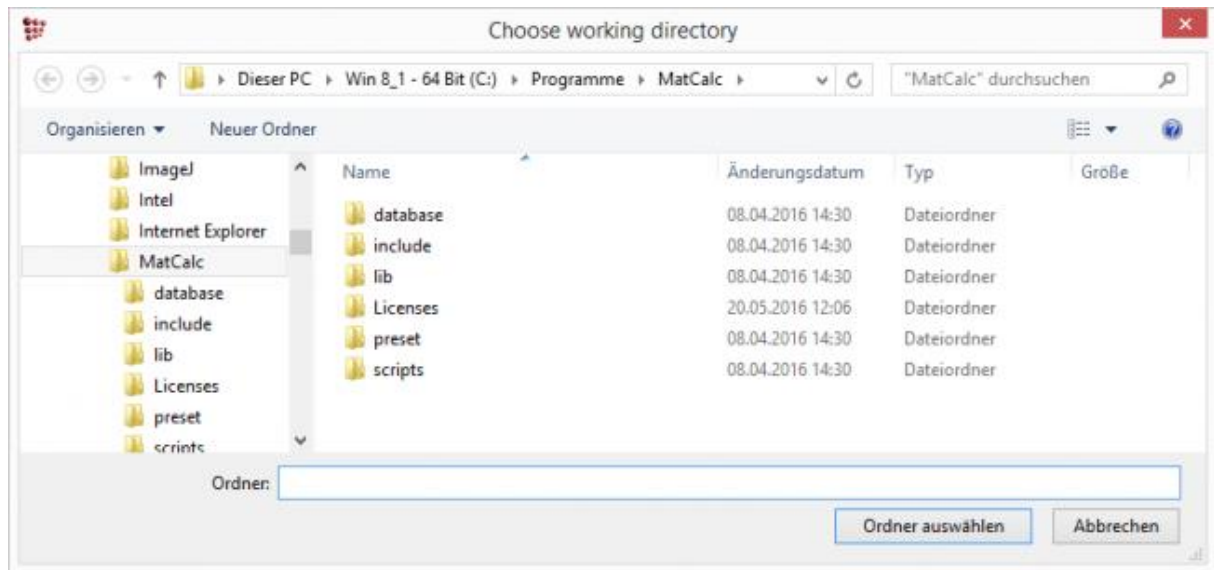


Select '**MatCalc workspace**' from the drop-box. This runs a script file called '**autonew.mcs**', which makes two additional windows appear: '**Phase details**' and '**Phase summary**'. When the new workspace is first created, the '**Phase summary**' and '**Phase details**' windows show messages indicating that no phases have yet been selected. The workspace is now ready for thermodynamic or precipitation calculations to be set up and performed.

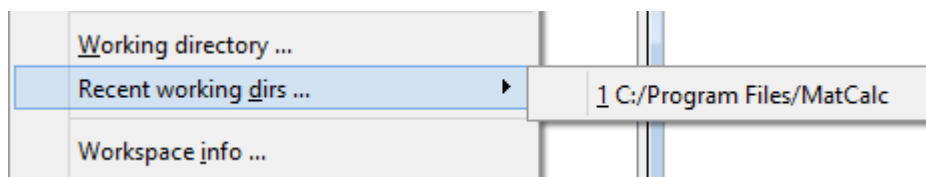


WORKING DIRECTORY

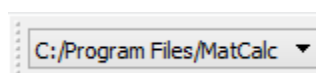
The '**working directory**' is the directory opened by default when saving new files or opening existing ones. Clicking on '**Working directory...**' allows the user to designate an existing directory as the working directory or to create a new directory for this purpose.



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.

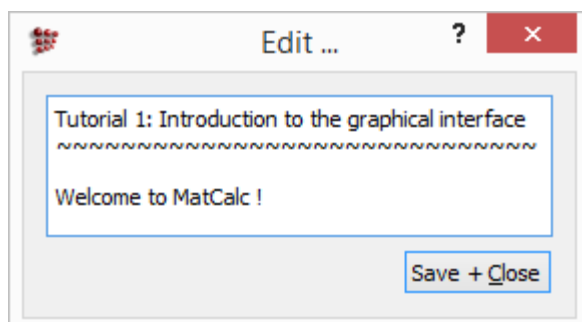


The same information is also available in a drop-box in the toolbar area:




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 in more detail in [Tutorial 12](#).

T2: CALCULATING A SINGLE EQUILIBRIUM

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

database: mc_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

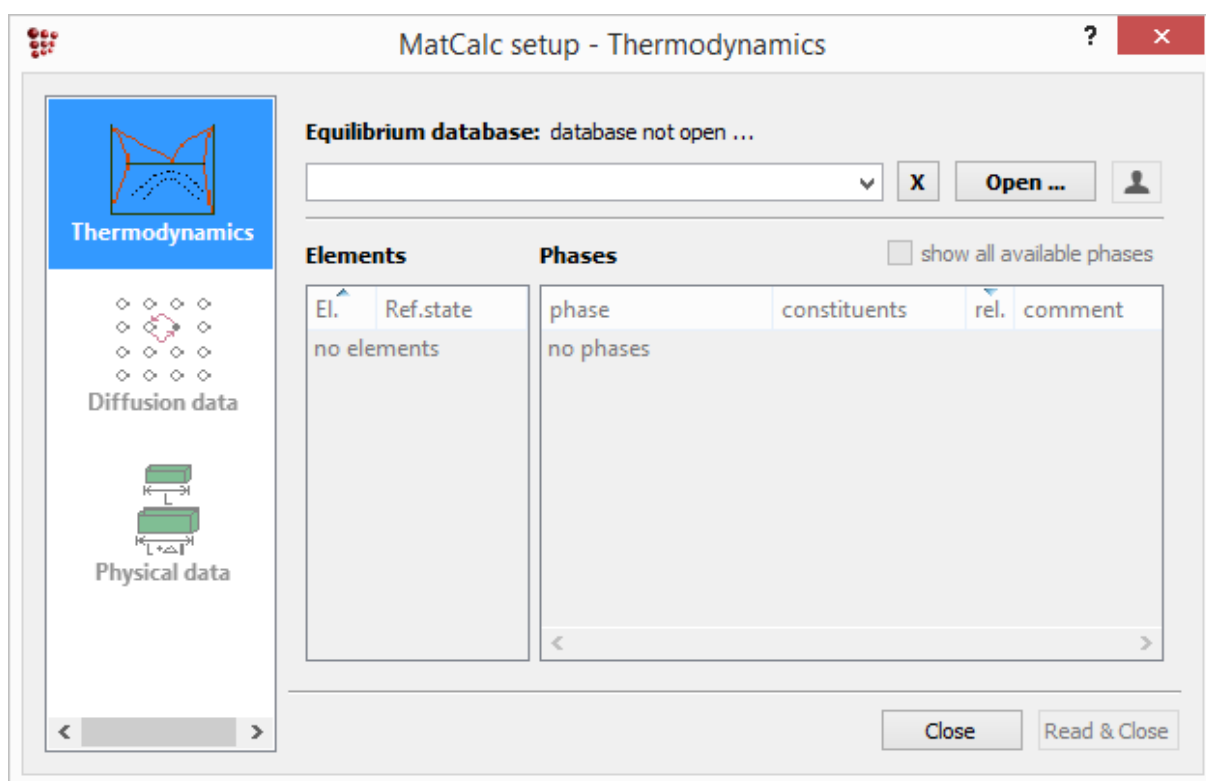
BEFORE STARTING...

Create a new workspace file ([Tutorial 1](#)).

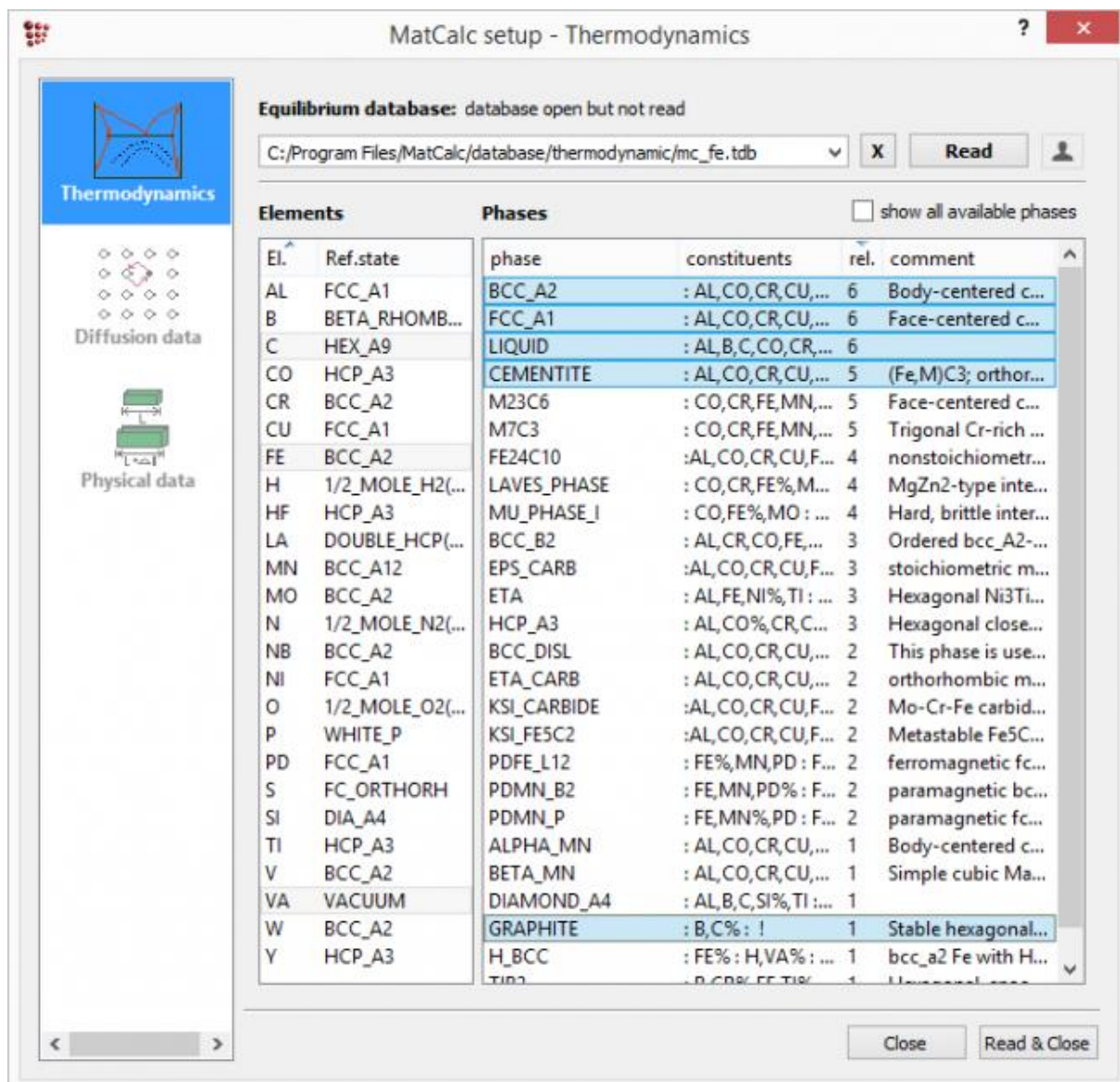
SETTING UP THE SYSTEM

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/thermodynamic**' subdirectory, allowing the user to choose a database. A small database on iron-based materials, '**mc_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**'.

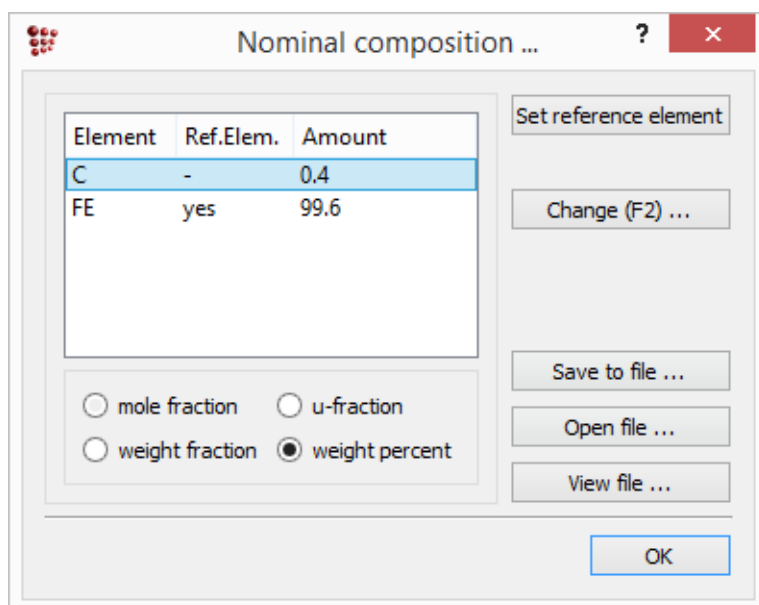


ENTERING THE COMPOSITION

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_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

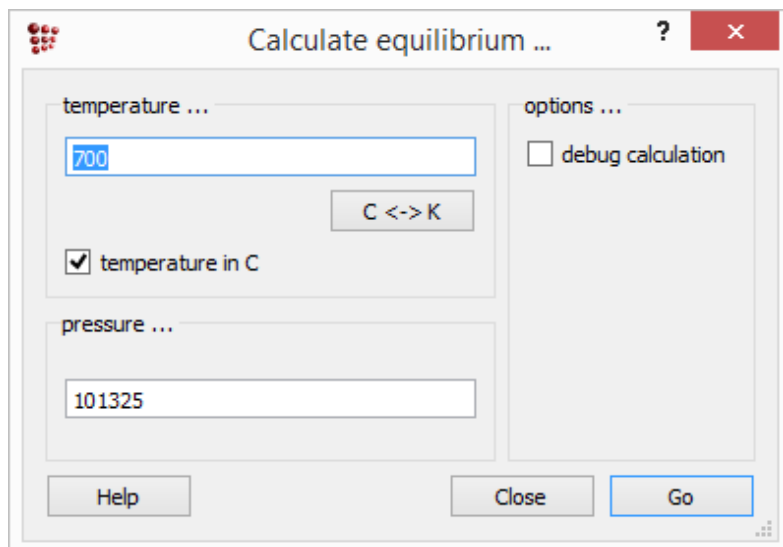
on the right, or by double-clicking in the '**Ref. Elem**' column by the side of the element name. To enter a composition of **0.4 wt.% C**, select '**weight percent**' as the unit, then highlight element C. Double-click in the '**Amount**' column, click on the '**Change**' button or press **F2** to 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 '**Console**', '**Phase status**' and '**Phase details**' windows each show information on the calculation which has just been performed. The final three lines of the console 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. Also the 'start' symbol on the Quick access menu is changed to the green check mark . 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. Moreover, the 'start' symbol in Quick Access menu will show a small warning sign .

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 console window or Quick Access menu before proceeding.

The other lines visible in the console window are messages relating to the opening and reading of the thermodynamic database.

```

MatCalc console

MatCalc defaults file (/preset/defaults.txt) version 2013-10-15

Checking for updates ...
Connecting to MatCalc Server ...
Ok
Your software is up-to-date.

mc_log file is disabled, use SET_LOG_FILE to enable it

<script(0/core)> $ phase details: create and move
<script(0/core)> new-gui-window a6
<script(0/core)> move-gui-window . 500 0 500 450move-gui-window window-id=. x-axis=500 y-axis=0 width=500 height=450

<script(0/core)> $ phase summary: create and move
<script(0/core)> new-gui-window a5
<script(0/core)> move-gui-window . 0 0 450 300move-gui-window window-id=. x-axis=0 y-axis=0 width=450 height=300

<script(0/core)> $ clear modified-flag
<script(0/core)> set-workspace-property m n
<script(0/core)> $ ready ...

script 'C:/Program Files/MatCalc/scripts/autonew.mcs' finished in 0,10 secs on Mo, 2016-07-25, 21:00:16

opening database 'C:/Program Files/MatCalc/database/thermodynamic/mc_fe.tdb' ...
- OK -

opening database 'C:/Program Files/MatCalc/database/thermodynamic/mc_fe.tdb' ...
reading thermodynamic data 'C:/Program Files/MatCalc/database/thermodynamic/mc_fe.tdb' ...

collecting symbols 'C:/Program Files/MatCalc/database/thermodynamic/mc_fe.tdb' ...

elements: VA C FPhases: LIQUID FCC_A1 BCC_A2 GRAPHITE CEMENTITE

Gibbs: 5 Phases / 0 Composition-Set(s) created
Gibbs: 32 functions linked ...
Gibbs: T = 1273.160000 K, P = 101325.000000 Pa, moles = 1

iter: 86, time used: 0,01 s
T: 700 C (973,16 K), GibbsEnergy: -39976,445 J
- OK -

core$

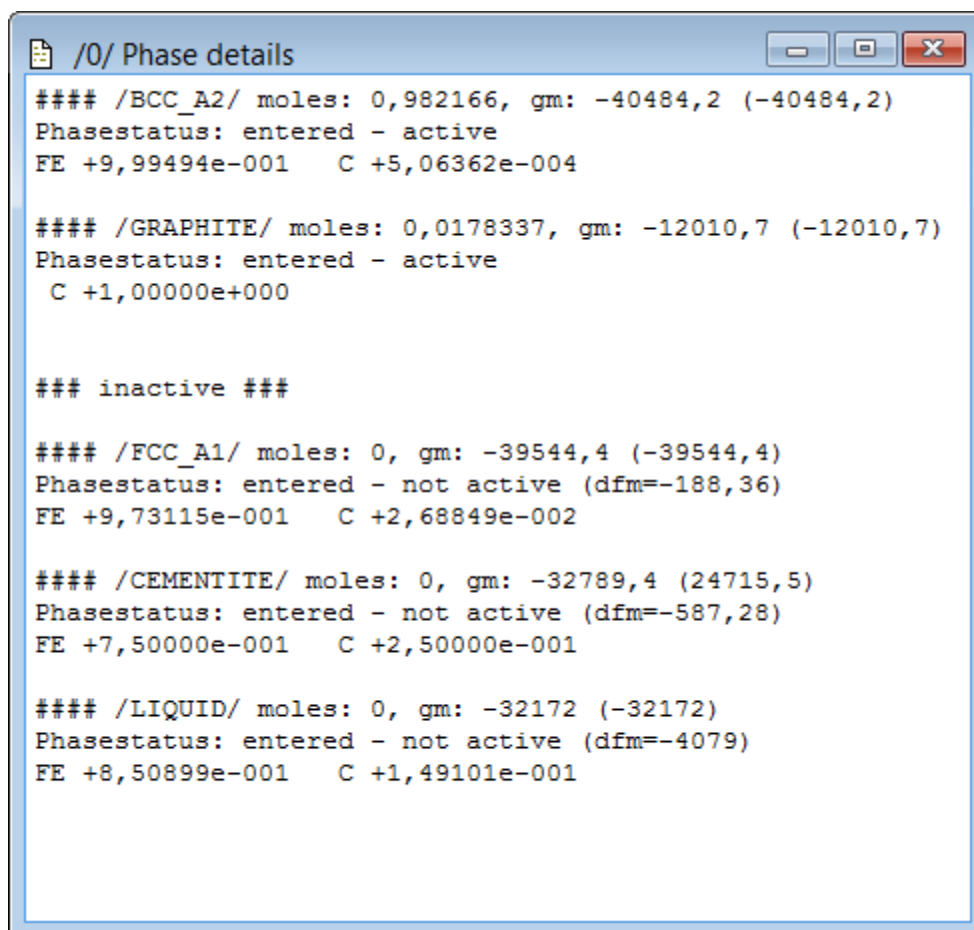
```

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.

/1/ Phase summary				
BCC_A2	*	act	9,82166e-001	dfm: +0,00000e+000
GRAPHITE		act	1,78337e-002	dfm: +0,00000e+000
### inactive ###				
FCC_A1		- OK -	0,00000e+000	dfm: -1,88360e+002
CEMENTITE		- OK -	0,00000e+000	dfm: -5,87283e+002
LIQUID		- OK -	0,00000e+000	dfm: -4,07902e+003

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)
Phasestatus: entered - active
FE +9,99494e-001 C +5,06362e-004

#### /GRAPHITE/ moles: 0,0178337, gm: -12010,7 (-12010,7)
Phasestatus: entered - active
C +1,00000e+000

### inactive ###

#### /FCC_A1/ moles: 0, gm: -39544,4 (-39544,4)
Phasestatus: entered - not active (dfm=-188,36)
FE +9,73115e-001 C +2,68849e-002

#### /CEMENTITE/ moles: 0, gm: -32789,4 (24715,5)
Phasestatus: entered - not active (dfm=-587,28)
FE +7,50000e-001 C +2,50000e-001

#### /LIQUID/ moles: 0, gm: -32172 (-32172)
Phasestatus: entered - not active (dfm=-4079)
FE +8,50899e-001 C +1,49101e-001
```

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 > Show options window**' or right-clicking in the toolbar area and selecting '**options**' from the menu.)

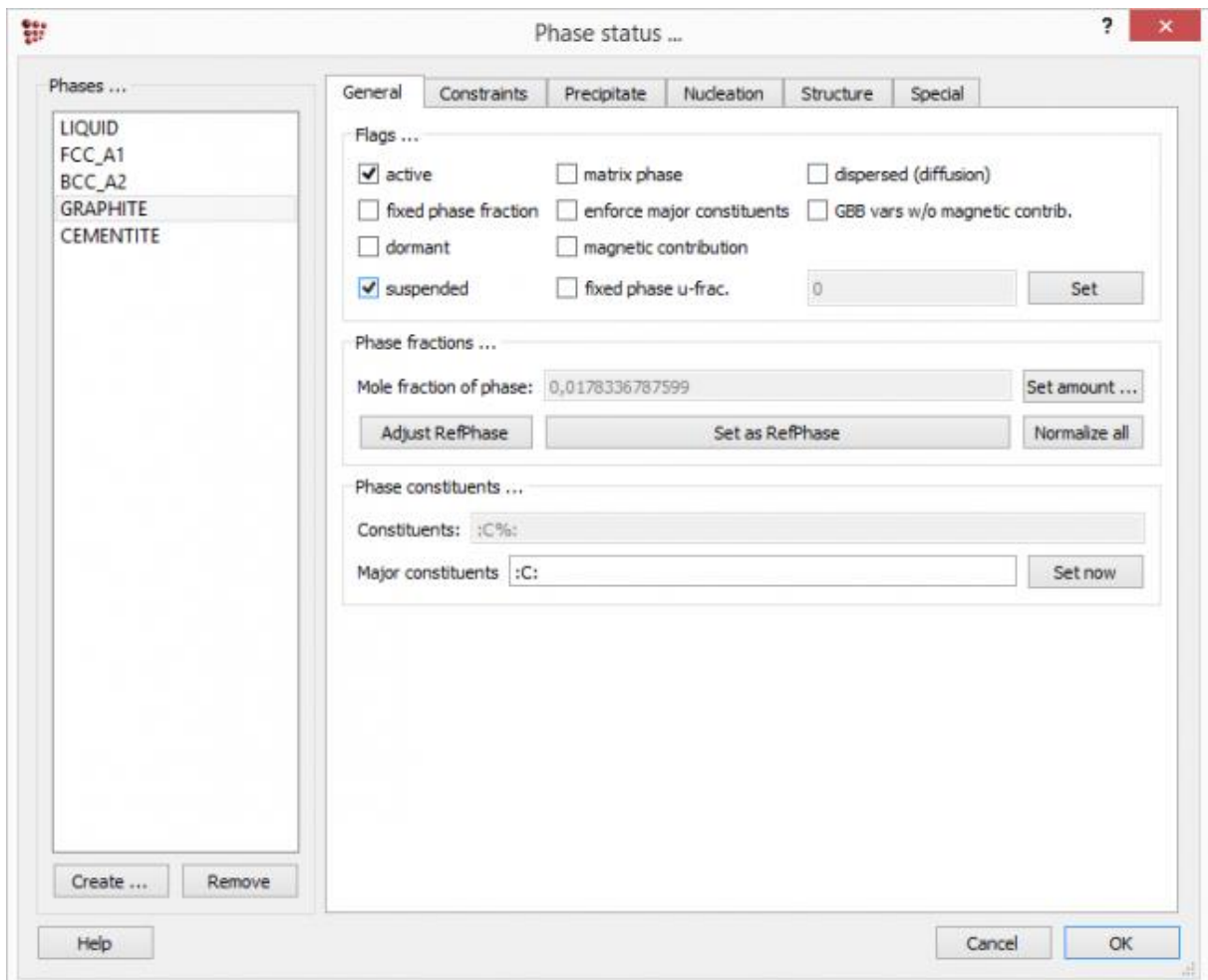
The '**Options**' window provides display options for the currently highlighted window. In the case of the '**Phase details**' window, the composition can be displayed as a mole fraction, a weight fraction or a u-fraction, and can also be expressed as a percentage if required.

options ...	
option	value
composition in	mole fraction
in percent	no

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**' and click '**OK**'.



Phase status ...

Phases ...

- LIQUID
- FCC_A1
- BCC_A2
- GRAPHITE
- CEMENTITE

Create ... Remove

Help

General Constraints Precipitate Nucleation Structure Special

Flags ...

- ☒ active
- ☐ fixed phase fraction
- ☐ dormant
- ☒ suspended
- ☐ matrix phase
- ☐ enforce major constituents
- ☐ magnetic contribution
- ☐ fixed phase u-fac.
- ☐ dispersed (diffusion)
- ☐ GBB vars w/o magnetic contrib.

0 Set

Phase fractions ...

Mole fraction of phase: 0,0178336787599 Set amount ...

Adjust RefPhase Set as RefPhase Normalize all

Phase constituents ...

Constituents: :C%:

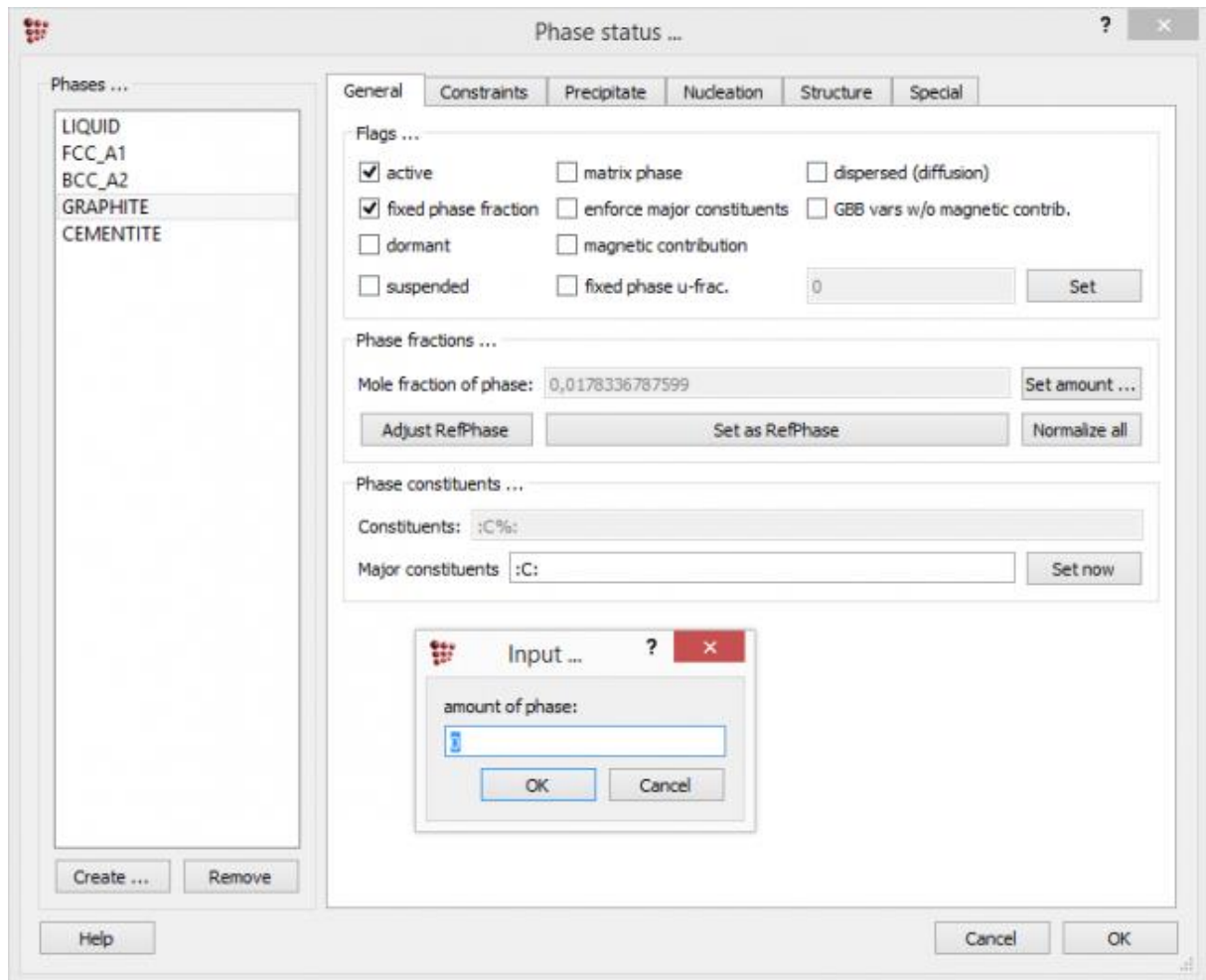
Major constituents :C: Set now

Cancel OK

Repeat the equilibrium calculation and note the difference in results in the 'Phase summary' window:

```
BCC_A2      *      act      9.29191-001      dfm: +0.00000e+000
CEMENTITE   act      7.08095-002      dfm: +0.00000e+000
### inactive ###
FCC_A1      - OK -      0.00000+000      dfm: -1.19178e+002
LIQUID      - OK -      0.00000+000      dfm: -3.71669e+003
### suspended ###
GRAPHITE
```

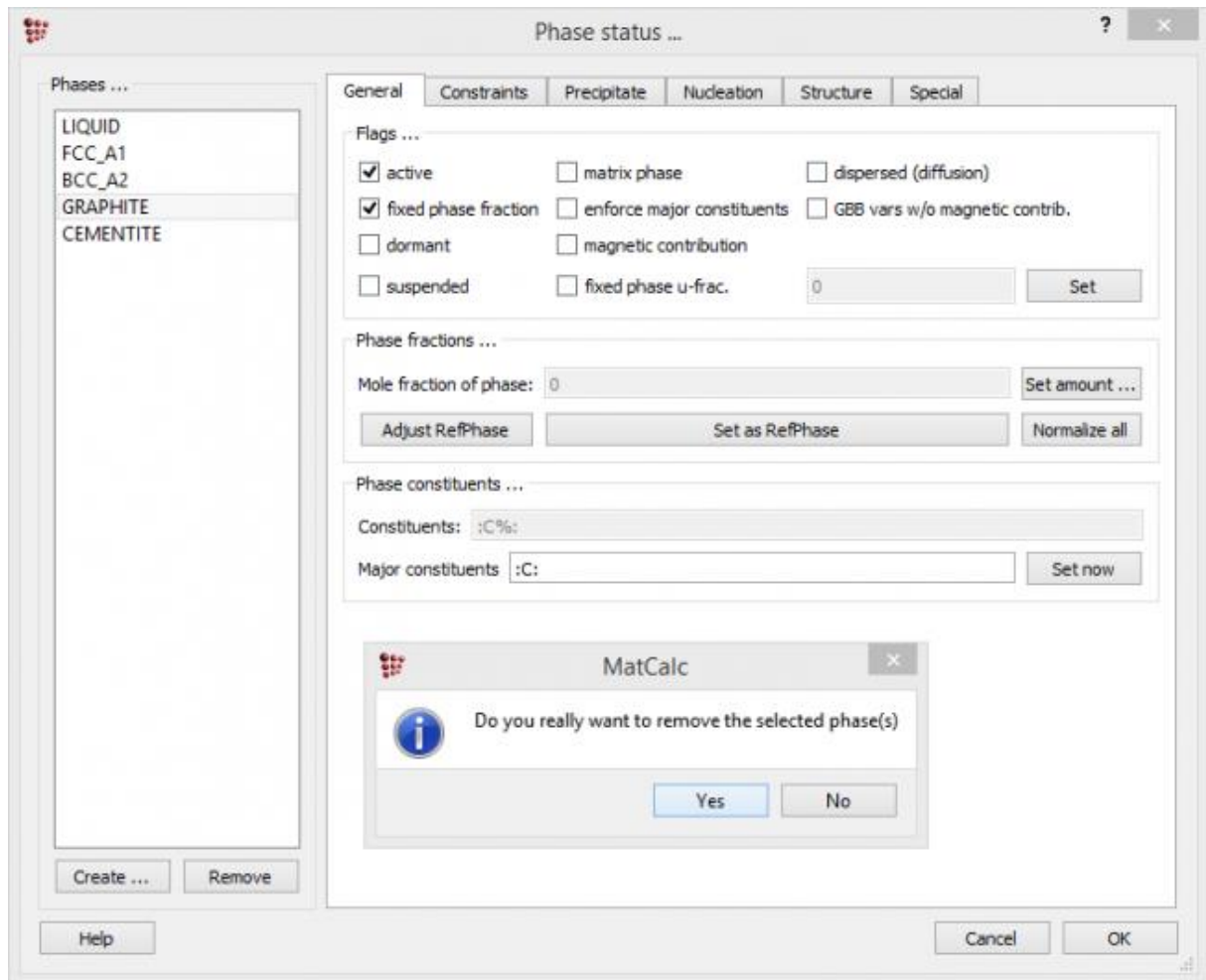
Now BCC_A2 and CEMENTITE are active, FCC_A1 and LIQUID are inactive and GRAPHITE is listed as '**suspended**'. Suspending a phase causes the program to consider it as if it were not there at all; the next most stable phase (in this case, cementite) becomes the equilibrium phase. Alternatively, the flag can be set to '**fixed phase fraction**' using the same procedure (i.e. in the 'General' tab of the 'Phase status' window, remove the tick from 'suspended' and place it in the 'fixed phase fraction' box for the graphite phase). Next, click on '**set amount...**' in 'Phase fractions' area and type '**0**' (zero) in the appearing '**Input...**' window.



Perform an equilibrium calculation again. In this case, the phase is considered not to appear, but its driving force is still evaluated. Also, cementite becomes active, as shown by the results below:

BCC_A2	*	act	9.82166-001	dfm: +0.00000e+000
CEMENTITE		act	7.08095-002	dfm: +0.00000e+000
### inactive ###				
GRAPHITE		fixed	0.00000+000	dfm: +2.35328e+003
FCC_A1	- OK -		0.00000+000	dfm: -1.19178e+002
LIQUID	- OK -		0.00000+000	dfm: -3.71669e+003

In order to eliminate graphite completely from the system, open the '**Phase status**' window, select the '**GRAPHITE**' phase and click on '**Remove**' button.



A new window will appear in which MatCalc will ask you to confirm this wish - click on **'Yes'**. Repeat the equilibrium calculation at 700°C to obtain an equilibrium without graphite. The driving forces obtained should be identical to those found in the previous calculation in which graphite was suspended:

```

BCC_A2      *      act      9.29191-001      dfm: +0.00000e+000
CEMENTITE   act      7.08095-002      dfm: +0.00000e+000
### inactive ###
FCC_A1      - OK -      0.00000+000      dfm: -1.19178e+002
LIQUID      - OK -      0.00000+000      dfm: -3.71669e+003
  
```

Adding any other phase to the system requires re-opening the thermodynamic database and selecting the new phase next to the already highlighted ones. Re-open **'Global > Databases'** and click on **GRAPHITE** to select 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 perform the

equilibrium calculation at 700°C once again to obtain an equilibrium with graphite (if you get an error message, click on '**Set start values**' in '**Calc**' menu). This time, the driving forces obtained should be identical to those found in the previous calculation in which graphite was present in the system:

```

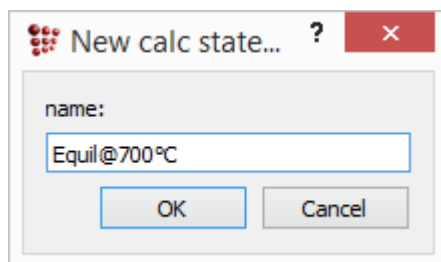
BCC_A2      *      act      9.82166-001      dfm: +0.00000e+000
GRAPHITE    act      1.78337-002      dfm: +0.00000e+000

### inactive ###

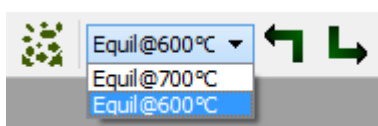
FCC_A1      - OK -      0.00000+000      dfm: -1.88360e+002
CEMENTITE   - OK -      0.00000+000      dfm: -5.87283e+002
LIQUID      - OK -      0.00000+000      dfm: -4.07902e+003
  
```



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 by creating 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**'.

T3: STEPPED EQUILIBRIUM CALCULATIONS

This tutorial was tested on
MatCalc version 6.00 rel 0.100
license: free
database: mc_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...

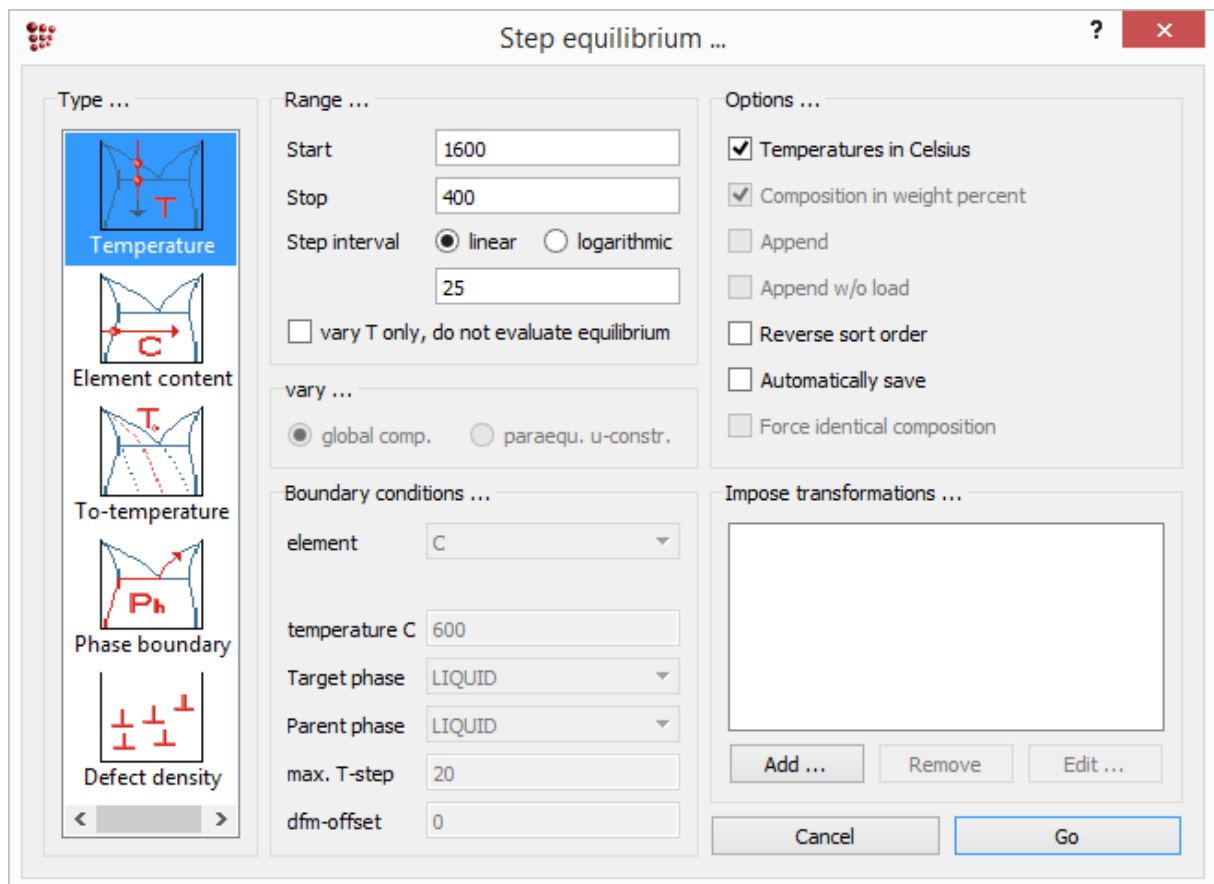
Re-open the file saved from [Tutorial 2](#) and load the calculation state '**Equil @ 600°C**'.

STEPPED EQUILIBRIUM CALCULATION WITH VARYING TEMPERATURE

RUNNING THE STEPPED CALCULATION

In phase status window, remove graphite phase. 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 '**console**' 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, 0.00 s, 725.00 C (998.16 K), its 4, BCC_A2 CEMENTITE - OK -
Tsol 'FCC_A1': 726.52 C (999.68 K) iter: 4, time used: 0.00 s
Tsol 'CEMENTITE': 726.52 C (999.68 K) iter: 5, time used: 0.00 s
7, 0.02 s, 750.00 C (1023.16 K), its 5, FCC_A1 BCC_A2 - OK -
8, 0.00 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, 0.00 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, 0.00 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, 0.00 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, 0.02 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: 0.00 s
37, 0.01 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, 0.00 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, 0.00 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, 0.00 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 -
Steps: 50, CalcTime: 0.25 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 726.52°C**, the two stable phases are **BCC_A2** (ferrite) and **CEMENTITE**. At **726.52°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 ...'**.

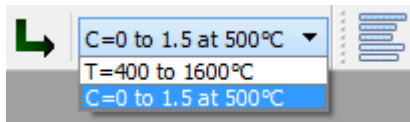
The final three lines of output give the number of steps and total calculation time, the current value of the stepped variable (673.16 K = 400°C) and an **'OK'** message indicating that the calculation was carried out successfully.

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, with each calculation state created in a different temperature. The default buffer is named **'_default_'**, and its contents are overwritten when a new stepped calculation is carried out.

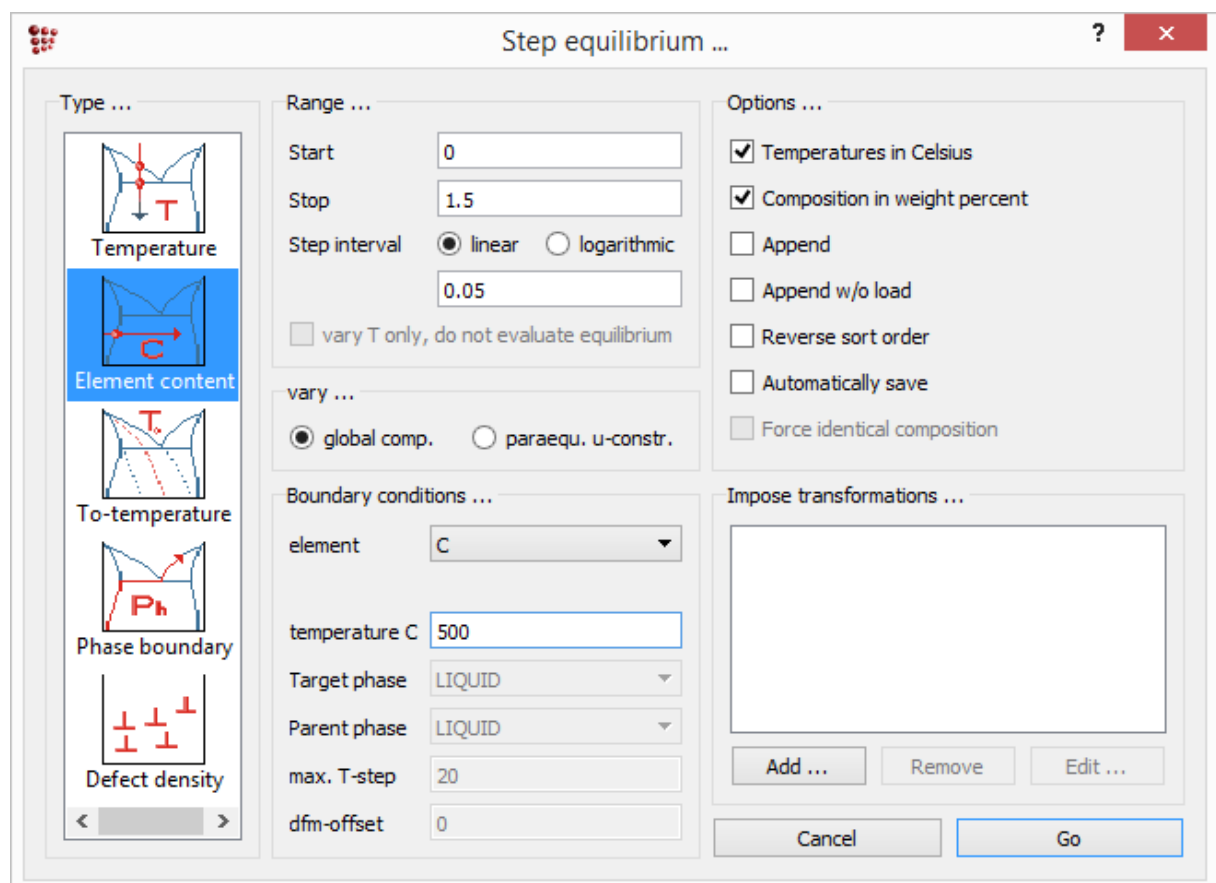
To be able to keep more than one set of stepped equilibria, additional buffers must be created. Firstly, rename the existing default buffer using **'Global > Buffers > Rename'**. Type **'T=400 to 1600°C'** into the **'New buffer name'** box and click **'OK'**. Then, create a new buffer using **'Global > 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 '**console**' 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): 5.7397782e-05, WP(C): 0.0012345083 - OK -
31, 0.00 s, 1e-12, its 4, BCC_A2 - OK -
```

```
Steps: 32, CalcTime: 0.11 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, 0,00 s, 0,4, its 74, 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, 0,00 s, 0,85, its 3, FCC_A1 - OK -
11, 0,00 s, 0,9, its 3, FCC_A1 - OK -
Xsol 'CEMENTITE': X(C): 0.042618502, WP(C): 0.9483187 - OK -
12, 0,00 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 -
```

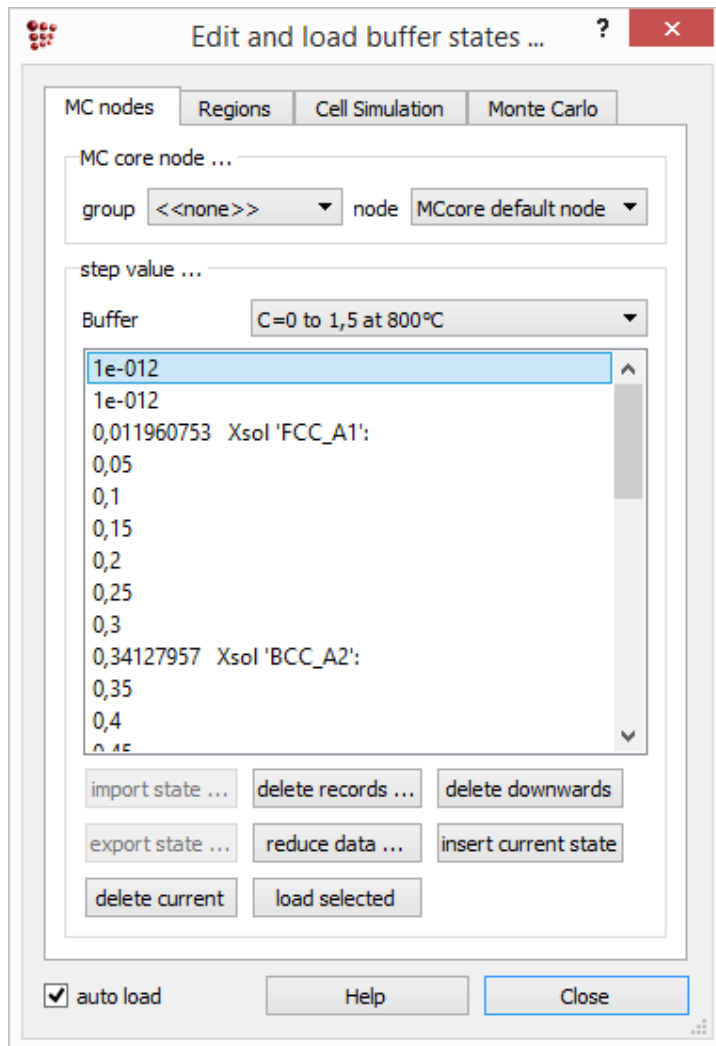
```

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 3, FCC_A1 - OK -
Xsol 'BCC_A2': X(C): 0.015673104, WP(C): 0.34127957 - OK -
25, 0,01 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-012, its 4, BCC_A2 - OK -
Steps: 32, CalcTime: 0,16 s
AktStepVal: 0,000000
- OK -

```

EDIT BUFFER STATES

The '**console**' 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 the 'step value' area 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](#).

T4: GRAPHICAL PRESENTATION AND EXPORT OF RESULTS

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

database: mc_fe.tdb


CONTENTS

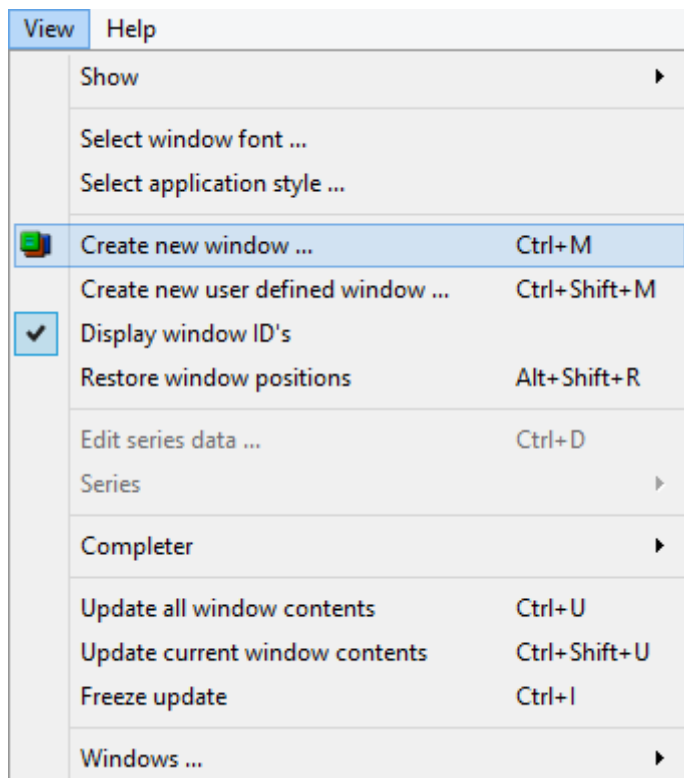
- Creating a new graphical window
- Introduction to the variables window
- Modifying the appearance of a plot using 'options'
- Zooming in and displaying x- and y-values
- Exporting a plot as an image and as numerical data

BEFORE STARTING...

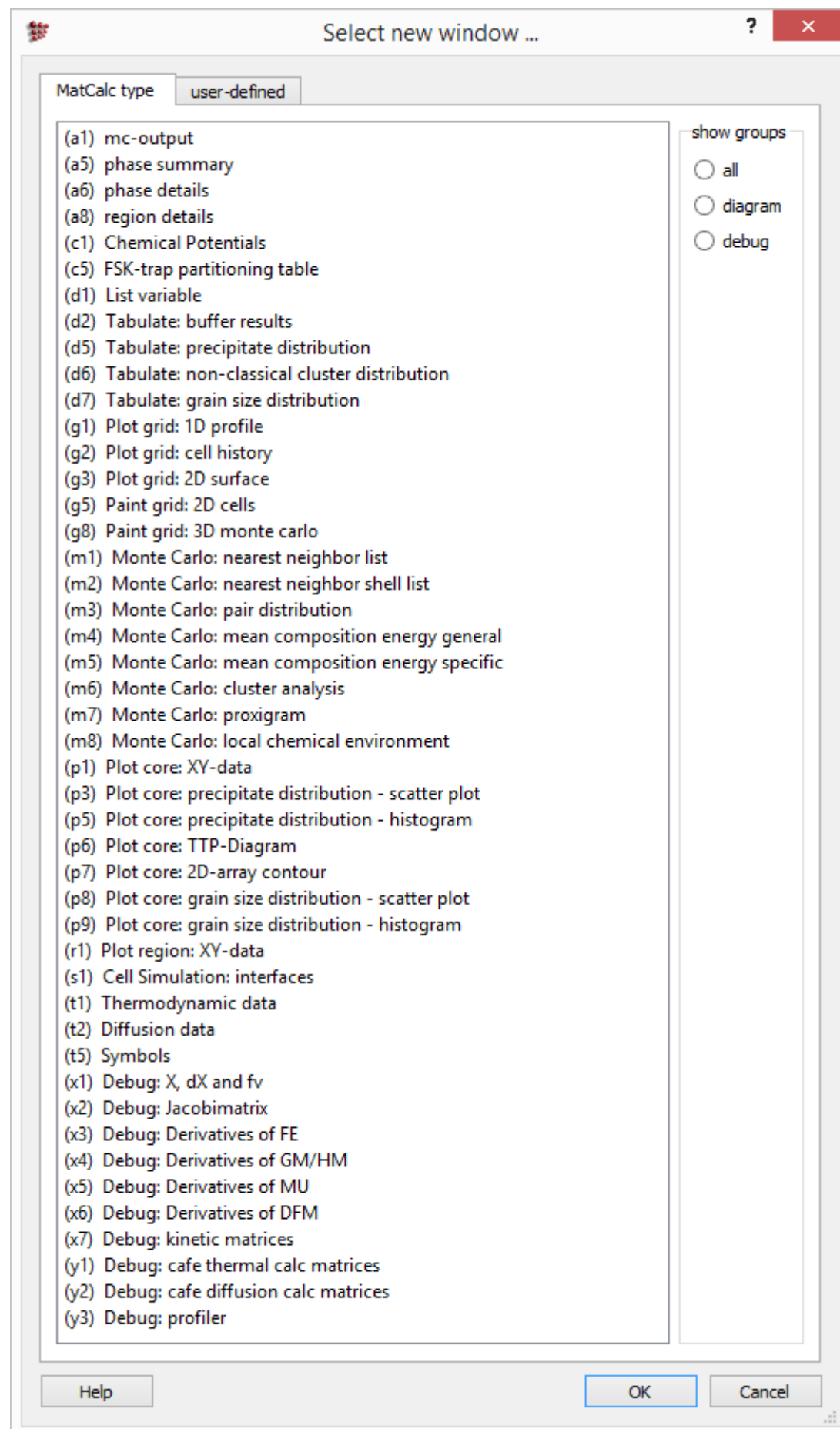
Open the file saved from [Tutorial 3](#) and select the buffer named '**T=400 to 1600°C**'.

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 '**(a5)**' and '**(a6)**', which are the familiar '**phase summary**' and '**phase details**' windows automatically placed on the screen when a new workspace file is created. Select type '**(p1) Plot core: XY-data**' and click on '**OK**'



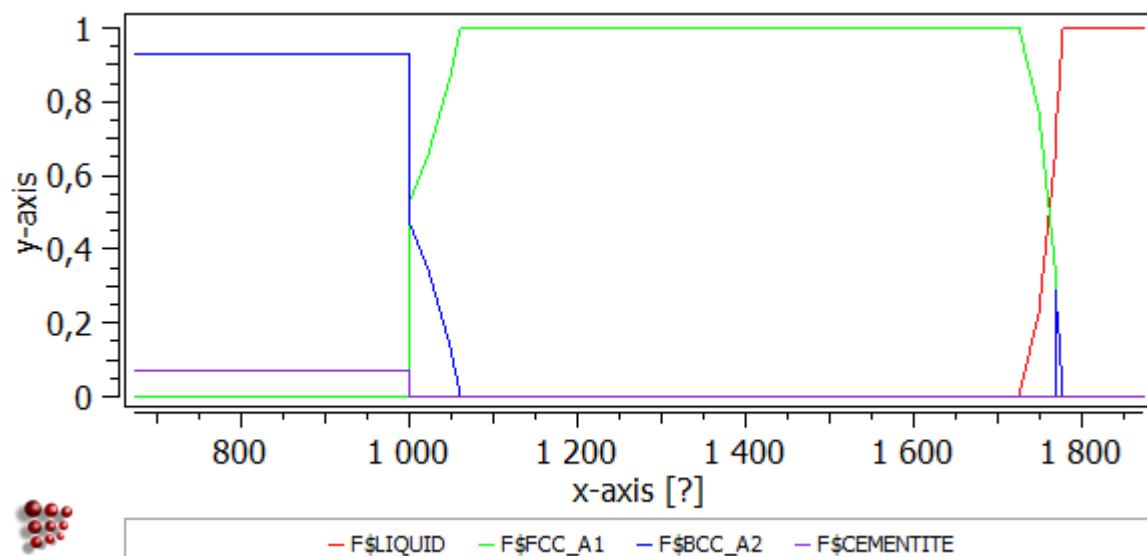
An empty plot with x- and y-axes appears on the screen. Locate the '**Variables**' window - if it is not present, right-click in the toolbar area at the top of the screen and select it from the menu,

or click on  icon in the '**Quick Access**' menu. 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.

variables	value
favorites	
T	1073.16
T\$ _c	800
StepValue	1e-12
F\$*	
F\$LIQUID	0
F\$FCC_A1	0
F\$BCC_A2	1
F\$CEMENTITE	0
X\$*X\$*	
X\$*X\$*X\$ _{wp}	
variables	
functions	
general	
phase fractions	

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:

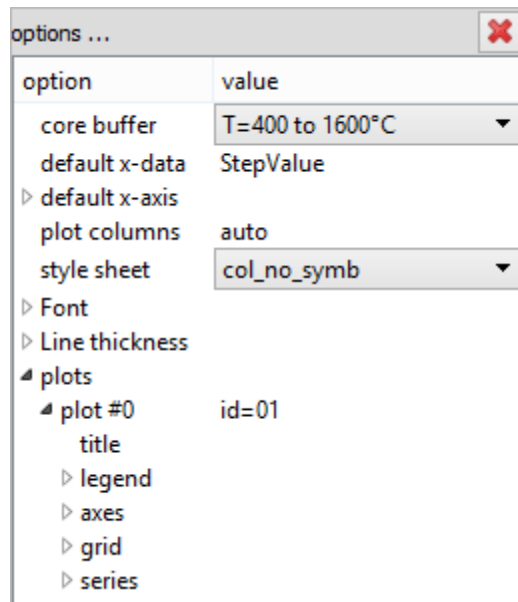


CHANGING THE APPEARANCE OF THE PLOT

RESULTS FROM DIFFERENT BUFFERS

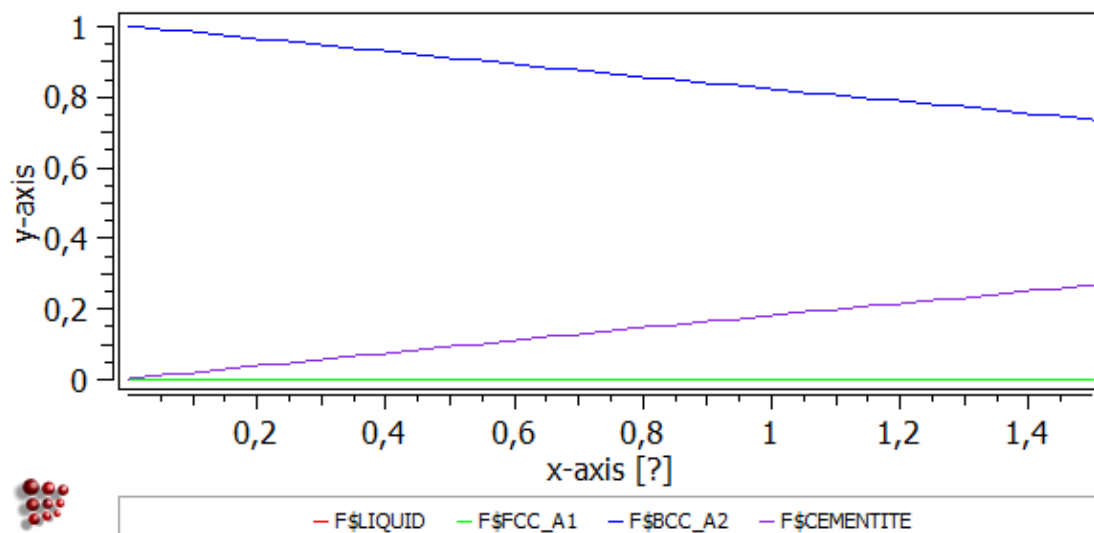
The '**Options**' window can now be used to modify the appearance of the plot as required.

(Again, if this is not currently shown, it can be made to appear by clicking on  icon in the Quick Access menu or the right-click menu in the toolbar area.)

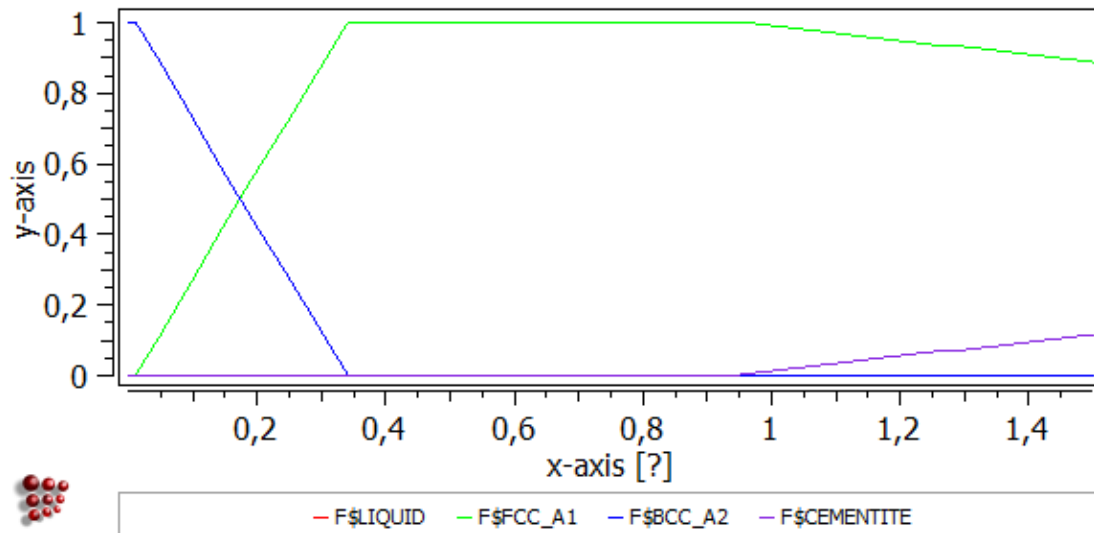


Firstly, note that there is a '**buffer**' drop-box. By selecting one of the other buffers, the contents of the plot can be changed. The '**default x-data**' option (the second line down in the options window) is set to StepValue, i.e. the value of the stepped variable used in the stepped equilibrium 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:

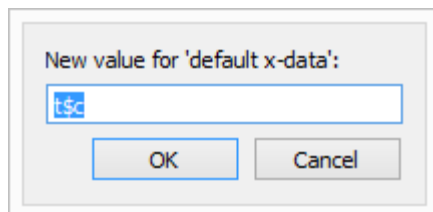


and the plot for the '**C=0 to 1.5 at 800°C**' buffer looks like this:



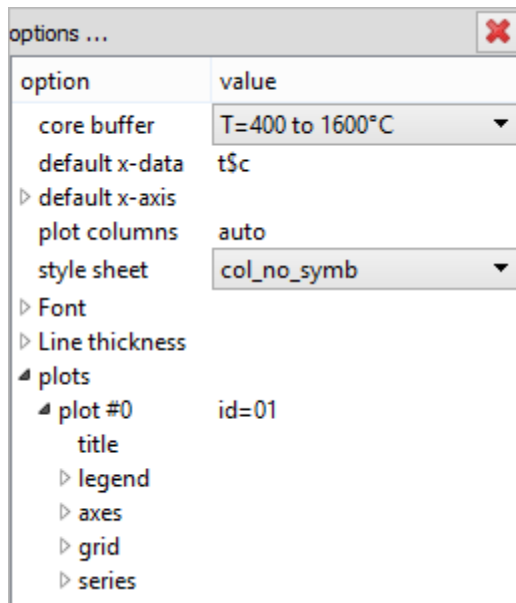
CHANGING THE FORMAT OF THE TEMPERATURE-STEP PLOT

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:

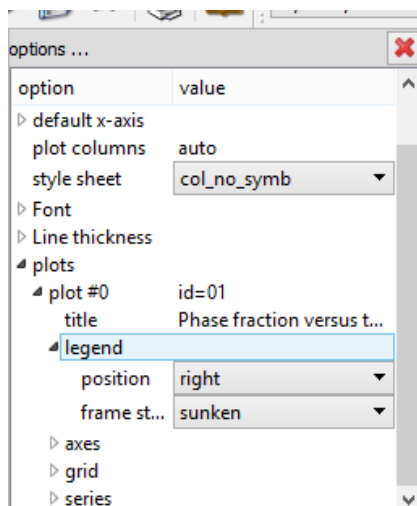


TITLE

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

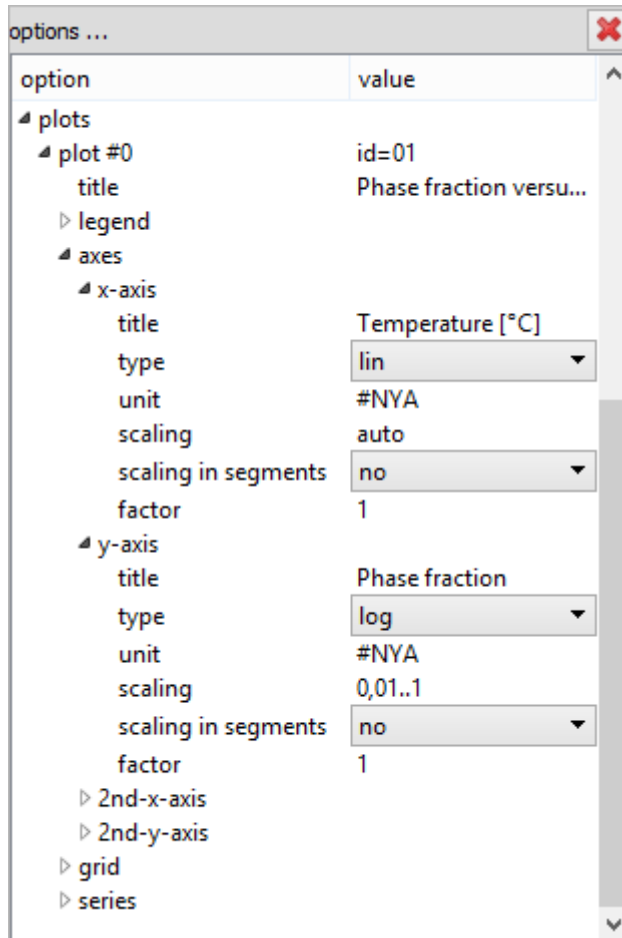
LEGEND

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 for **x-axis** 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 $F\delta^*$).

The changes on the x-axis properties will be visible only when the **'use for all plots'** setting at **'default x-axis'** is set to **'no'**. More information about the 'default x-axis' concept will be given in the next tutorial.

option	value
core buffer	T=400 to 1600°C
default x-data	StepValue
default x-axis	
use for all plots	no
title	x-axis [?]
type	lin
unit	#NYA
scaling	auto
factor	1
legend position	bottom

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
plots	
plot #0	id=01
title	Phase fraction vers...
legend	
axes	
grid	
major-x	enabled
minor-x	disabled
major-y	enabled
minor-y	disabled
major-pen	dot
major-color	none
minor-pen	dot
minor-color	none
series	

SERIES

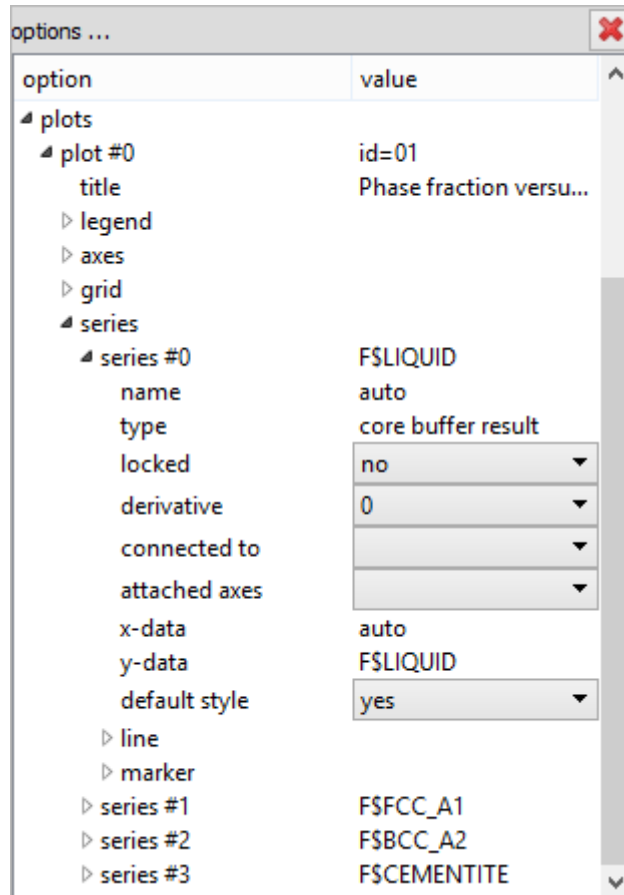
Expanding the **'series'** section gives a list of options for each data-series. The name of the series (as it appears in the legend) can be changed using **'name'**.

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.

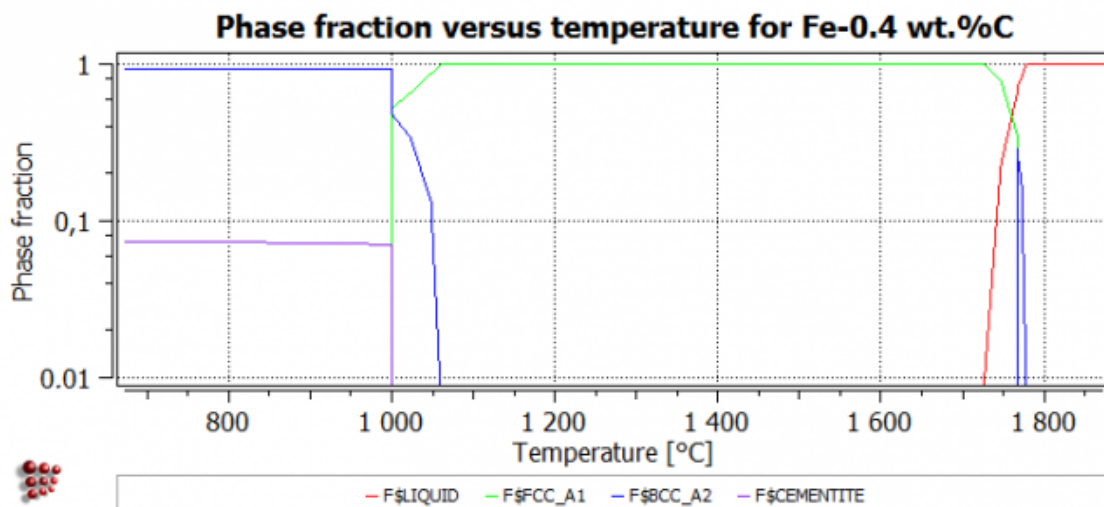
'Derivative' can be used to display the numerically evaluated first or second derivative of a series.

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

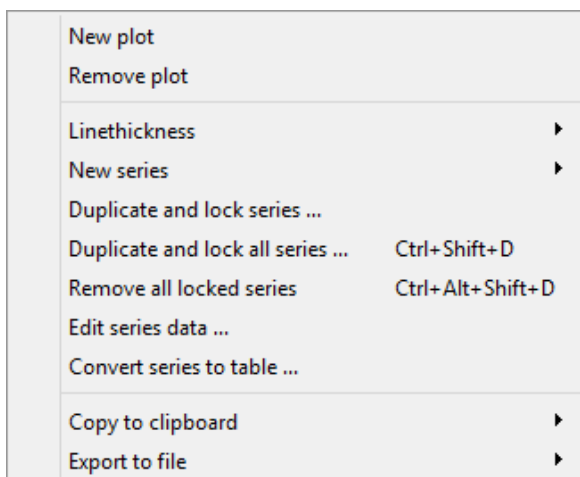
Left-click in the plot area and drag the mouse to draw a rectangular box. When the mouse button is released, an enlarged version of the region within the box is shown on the axes. Right-click anywhere in the plot area to return to the original scale.

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 this single plot or the whole frame (i.e. all plots in this window) in the **pixmap** (.bmp) or scalar vector graphics (**.svg**) format. Then the exported piece can be pasted to the relevant graphical application. Additionally 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 or the whole frame. The possible output file formats are '**.png**', '**.svg**' and '**.pdf**'

TO FINISH...

Save the workspace file.

T5: MATCALC BUILT-IN VARIABLES; GRAPHICAL OUTPUT

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

database: mc_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

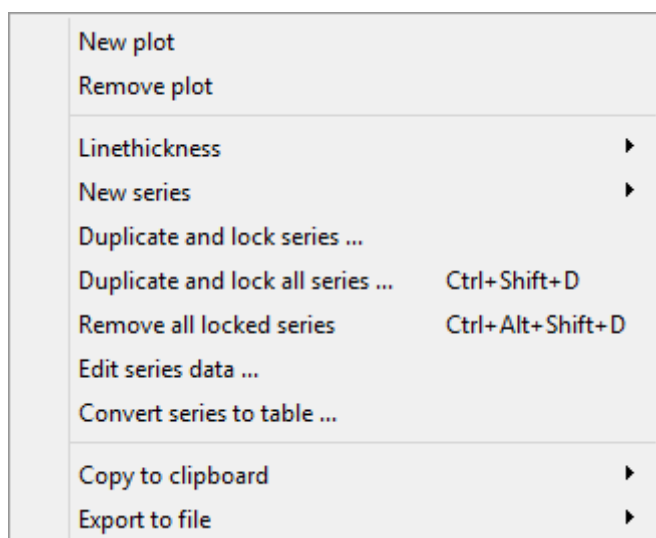
BEFORE STARTING...

Re-open the file saved in [Tutorial 4](#) and save it under a new name.

ADDING PLOTS OF DIFFERENT VARIABLES

CREATING A NEW PLOT

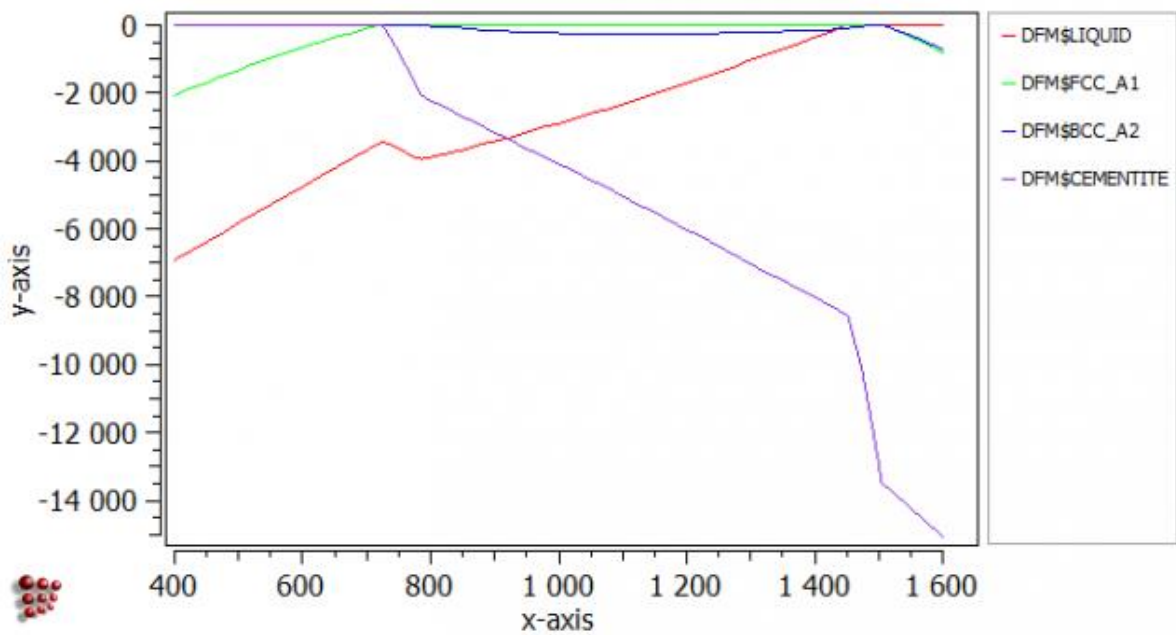
Highlight the plot window and right-click in this window outside the plot area to bring up the plot context menu already seen in Tutorial 4. Click on **'New plot'**.



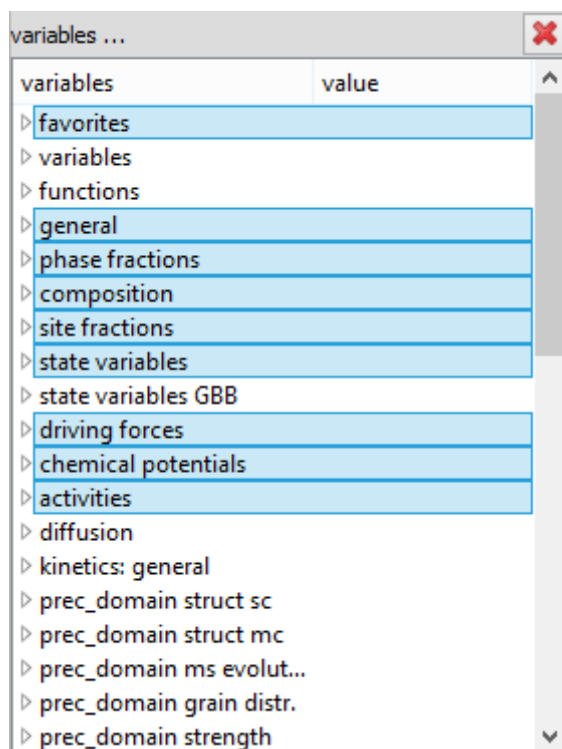
An empty plot appears below the original one.

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:



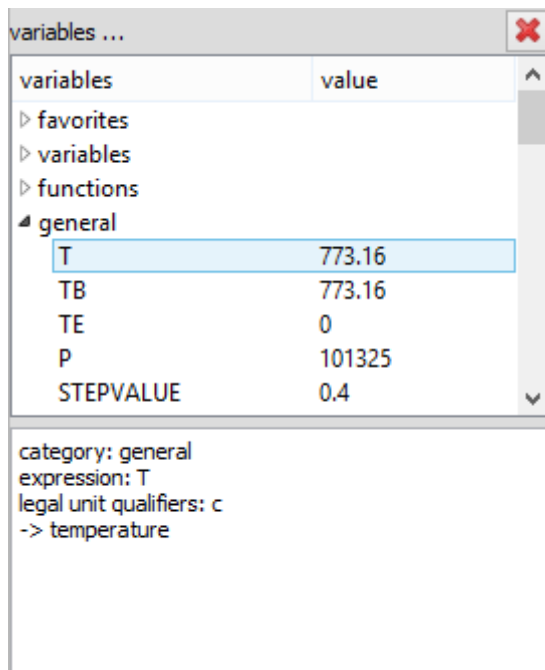
- 'FAVORITES'

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:



variables	value
▶ favorites	
▶ variables	
▶ functions	
▲ general	
T	773.16
TB	773.16
TE	0
P	101325
STEPVALUE	0.4

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, e.g. 'XPR\$*\$*' 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 '**Y\$BCC_A2\$FE\$0**' (site fraction of iron on sublattice 0) and '**Y\$BCC_A2\$C\$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'

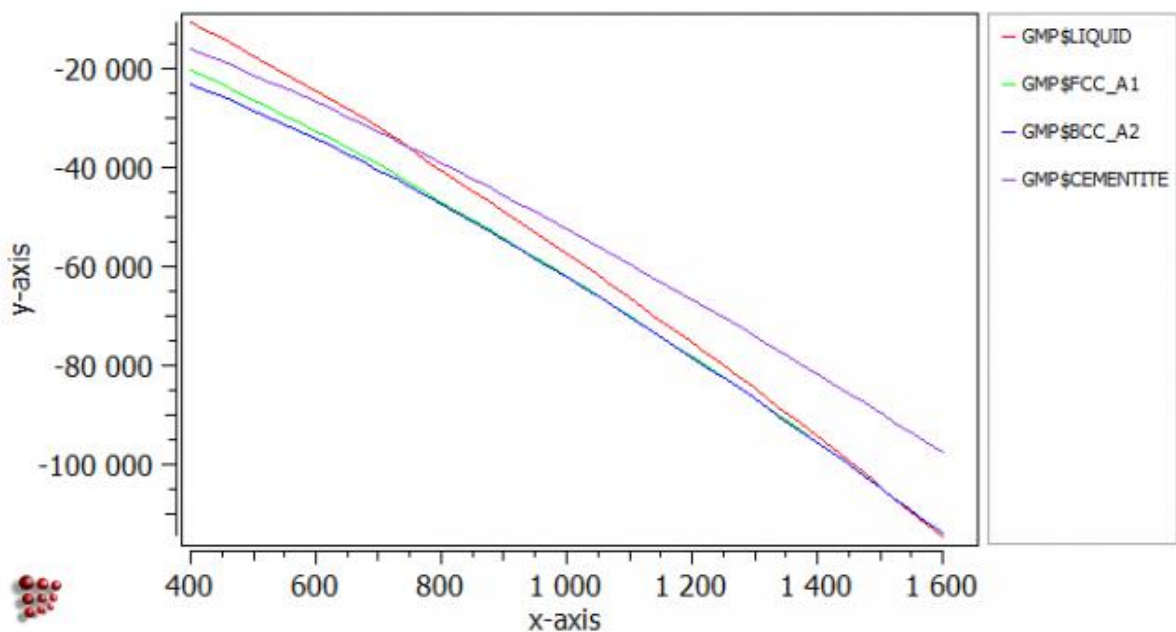
This category consists of a number of thermodynamic variables, including molar Gibbs free energies, entropies, enthalpies and heat capacities of the system and of each phase.

- 'CHEMICAL POTENTIALS', 'ACTIVITIES'

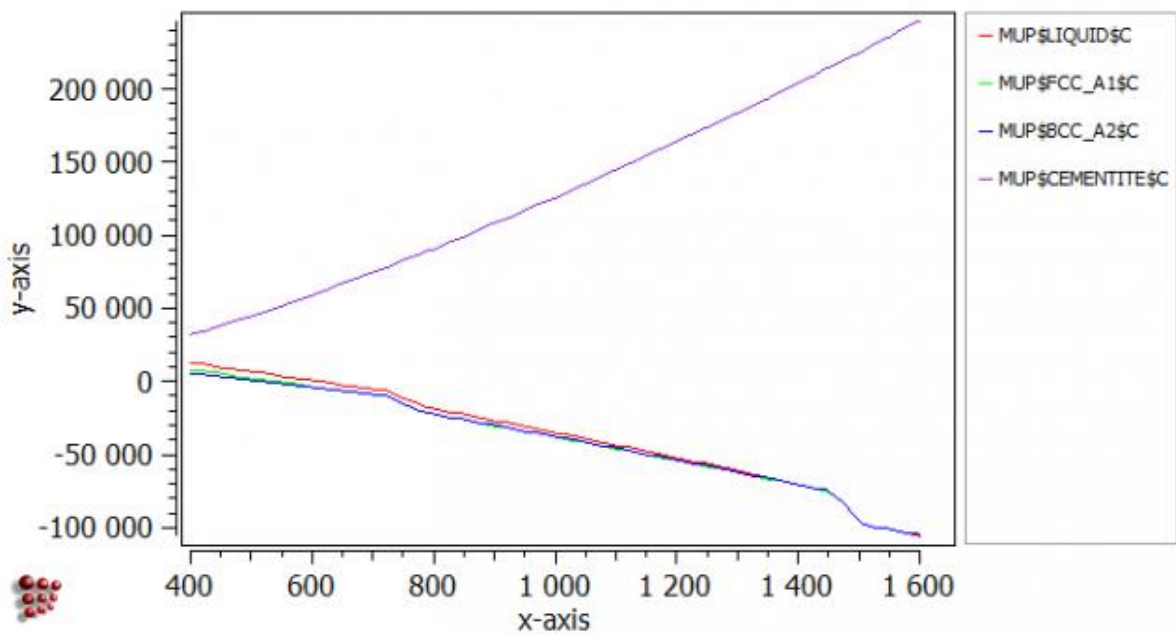
These categories include chemical potentials '**MU\$*****', activities '**AC\$*****' and activity coefficients '**ACC\$*****'.

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:

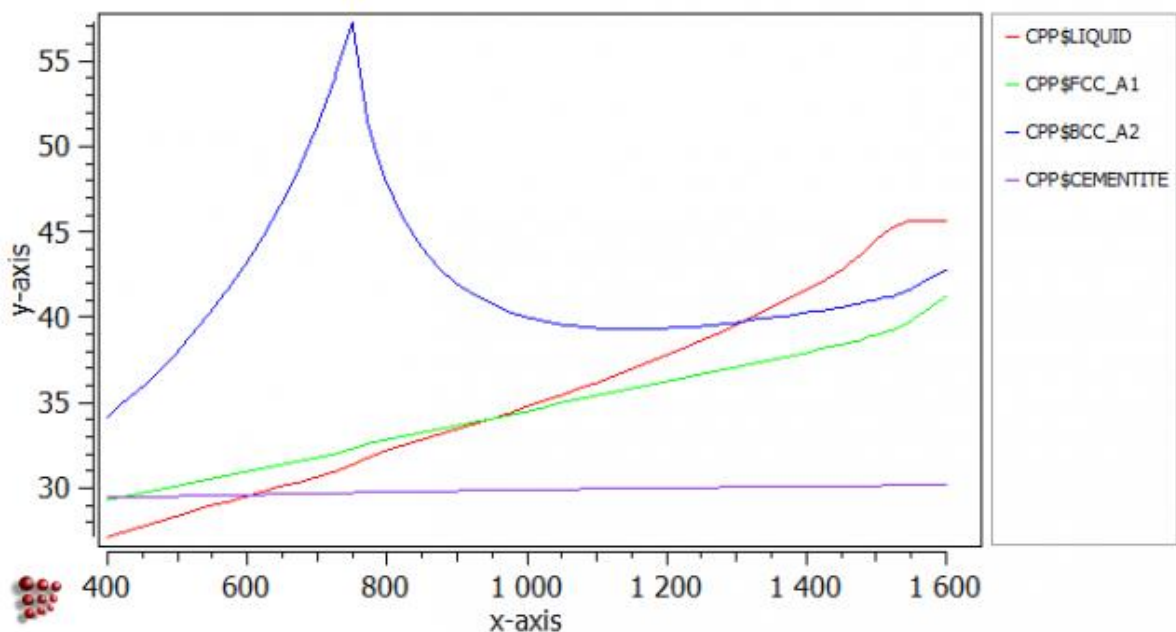
- Molar Gibbs free energy ('**GMP\$***')



- Chemical potential of carbon ('**MUP\$*C**')

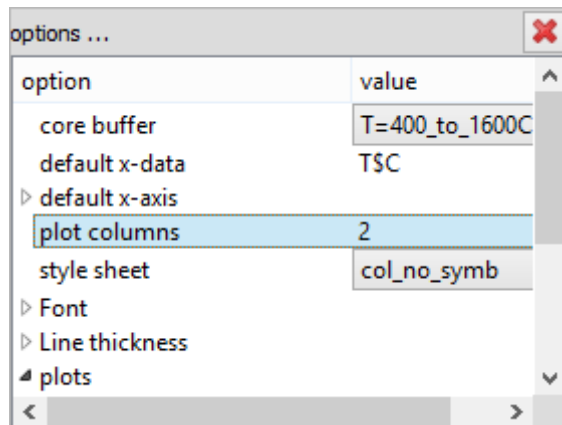


- Molar heat capacity ('**CPP\$***'), note the lambda-anomaly at the Curie temperature in BCC_A2)



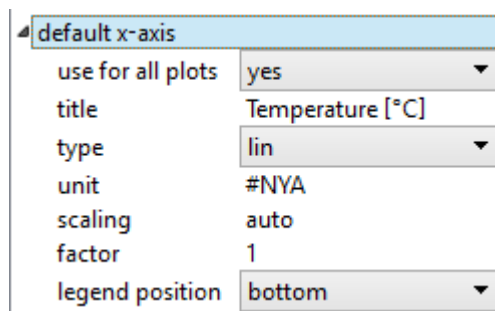
ARRANGING PLOTS IN THE COLUMNS

When there are many plots in the plot window then they will get stretched 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.



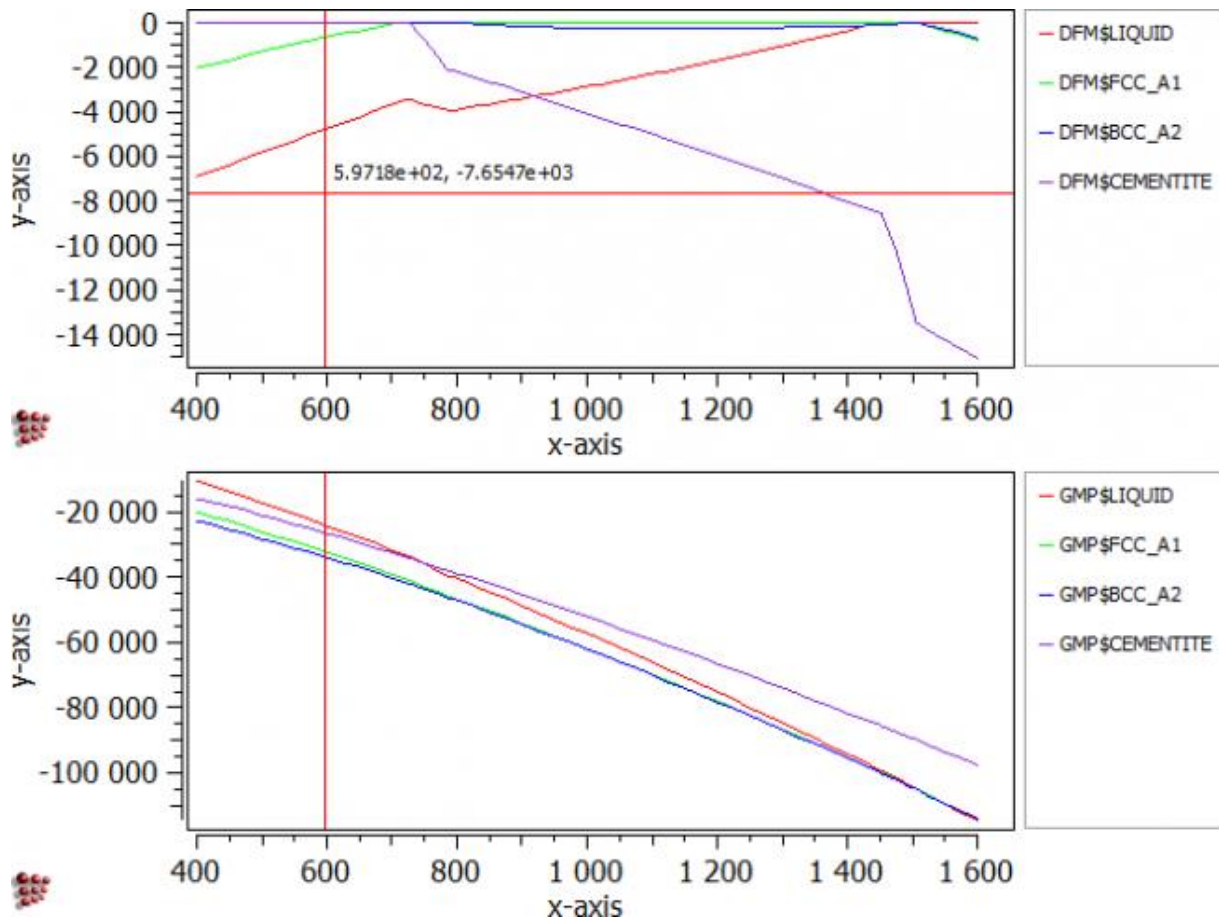
DEFAULT X-AXIS

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.



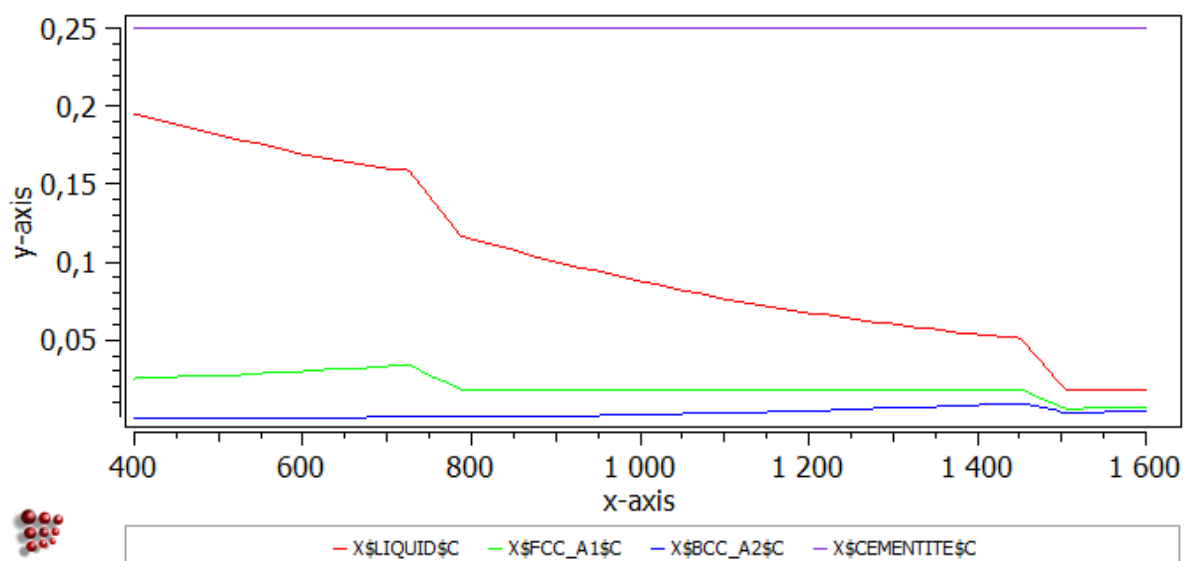
DISPLAYING X-VALUES OF MULTIPLE PLOTS

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:

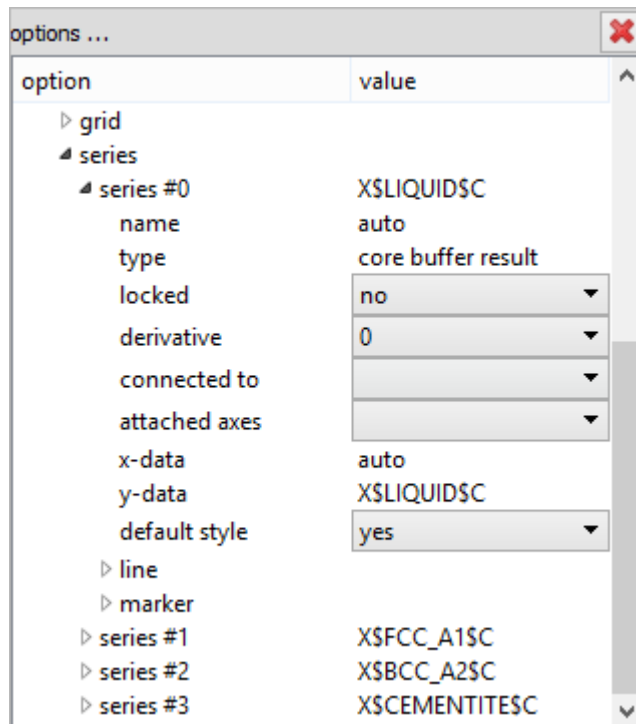


MODIFYING THE SERIES IN A PLOT

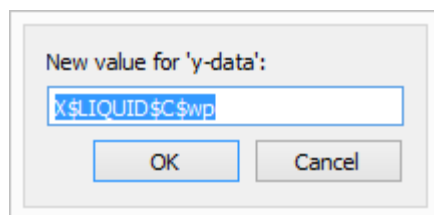
This part of the tutorial will demonstrate how to use the unit qualifiers mentioned above. Add a new plot to the plot window and drag and drop '**X\$*%C**' (carbon content of the phases) from the '**variables**' window. The resulting plot should look like this:



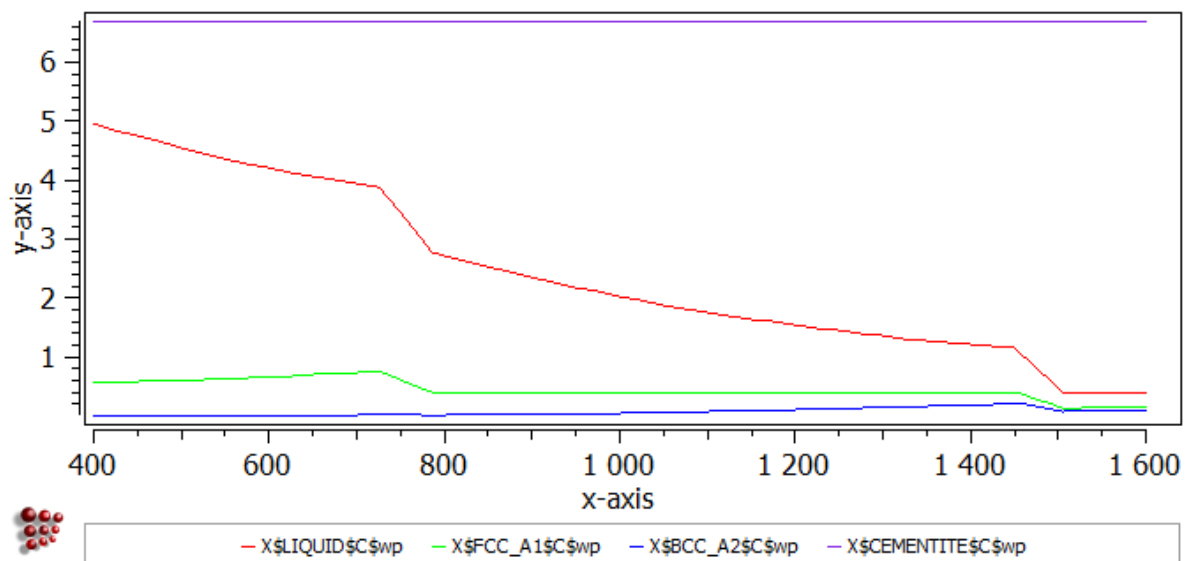
By default, the carbon content is expressed in mole fraction. To change the units to weight percent, firstly click on the new plot to select it. This should expand the section of the '**Options**' list which applies to the new plot. Click on the triangle by '**series**' to open the series options:



Double-click on '**y-data**' for the first series to open the following box. Append '**\$wp**' to the existing expression and click '**OK**'.

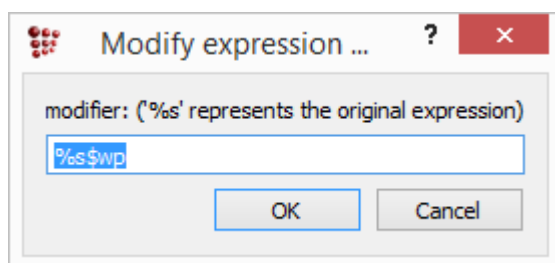


This will change the values plotted for the '**LIQUID**' series. Repeat for the other three series. The final appearance of the plot, with appropriate axis labels added, should be as shown below.



MODIFYING THE SERIES WITH DRAG AND DROP

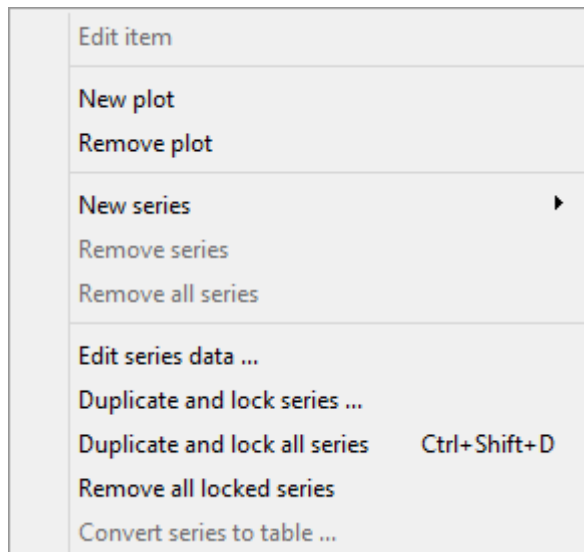
Alternatively you can select the variable and drag it to the window, and press **'Ctrl'** before dropping it to the plot. An option window will pop up, where you can modify the original expression (read as %s) by adding mathematical operations or **change it to weight percent** by **appending '\$wp'**.



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.

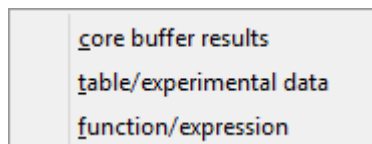
OTHER SERIES OPERATIONS

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

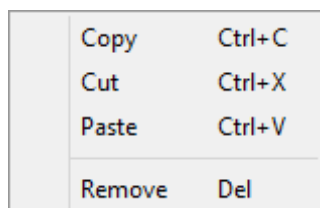


- 'NEW SERIES'

The '**New series**' part of the menu expands to give the following sub-menu (provided that a plot is selected).



Clicking on '**core 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:

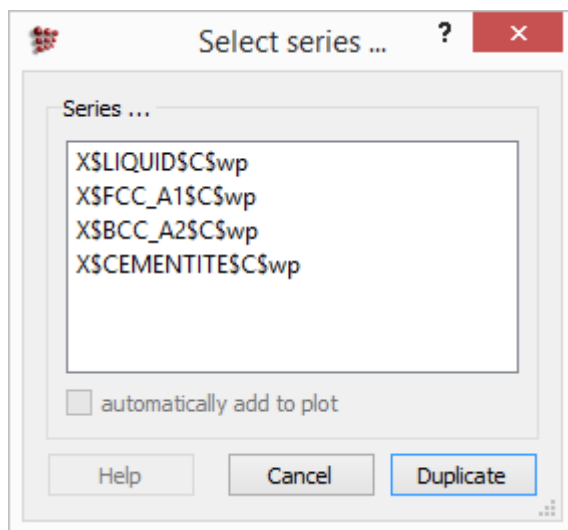
- '**table/experimental data**': allows the user to add a set of experimental data points to a plot.
- '**function/expression**': enables an algebraic expression in (x) to be entered.

- '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'

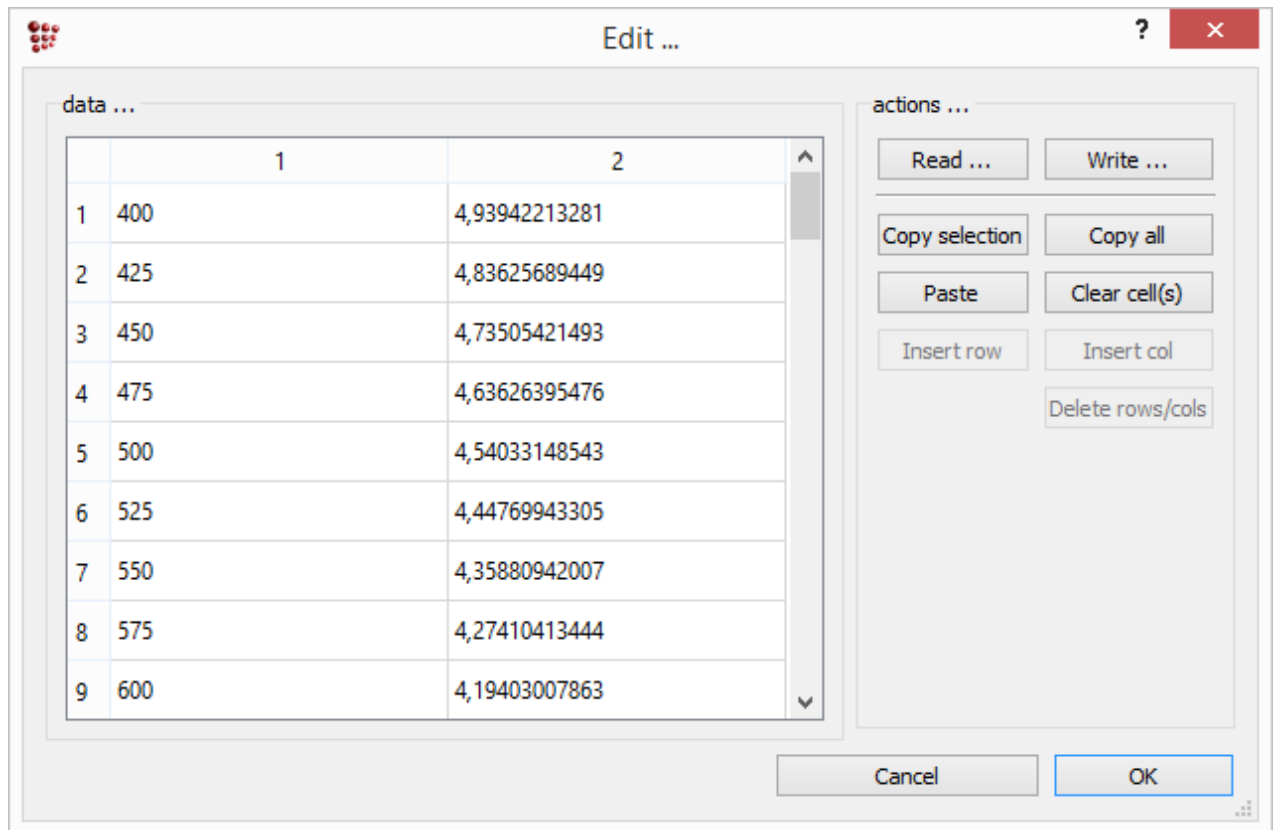
This feature is available in the right-click menus of both the Options window and the plot window. Click on **'Duplicate and lock series'**, select a series from the list shown and click on **'Duplicate'** button. This will lock the original series and create a copy.



'Duplicate and lock all series' performs this operation for all series in the selected plot window. The locked series is protected from any changes when the buffer contents are updated with new calculation results, while the copy is unlocked. This enables an 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 in the appearing window and click on **'Edit...'** to display a table containing the numerical data used to plot the graph.

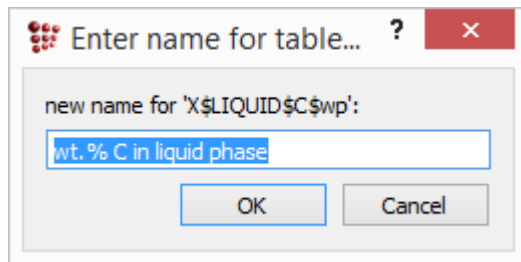


The data can be copied using the **'Copy selection'** or **'Copy all'** buttons. The contents of the rows and columns can be modified using **'Paste'** (to add data copied from another source), **'Clear cell(s)'**, **'Insert row'**, **'Insert col'** and **'Delete rows/cols'** buttons. Use **'Write'** to save the whole dataset to a text file and **'Read'** to load a dataset from a text file.

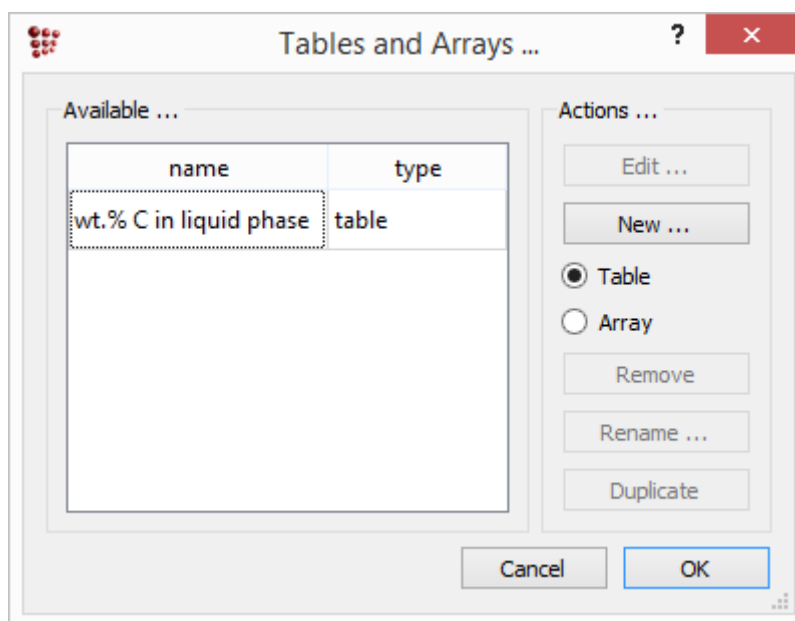
- 'CONVERT SERIES TO TABLE'

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

Select the **'series'** in **'Options'** window, 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.



T6: INTRODUCTION TO USER-DEFINED FUNCTIONS AND VARIABLES

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

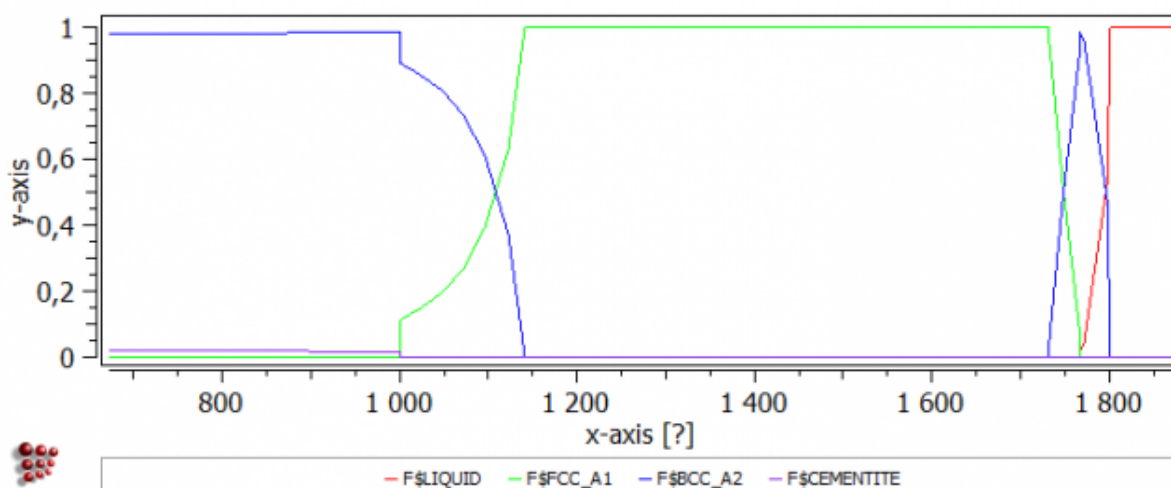
database: mc_fe.tdb

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 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]**'.

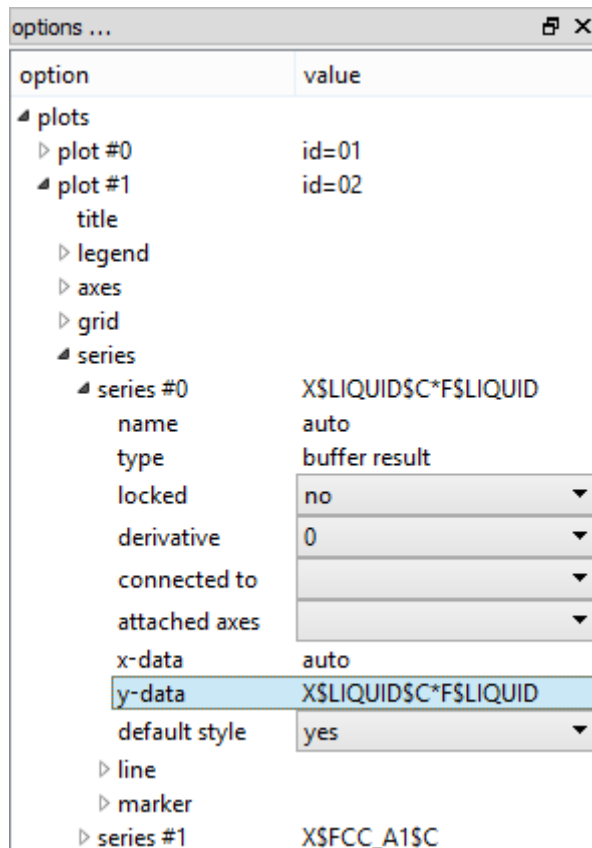
COMBINING BUILT-IN VARIABLES IN NEW EXPRESSIONS

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.

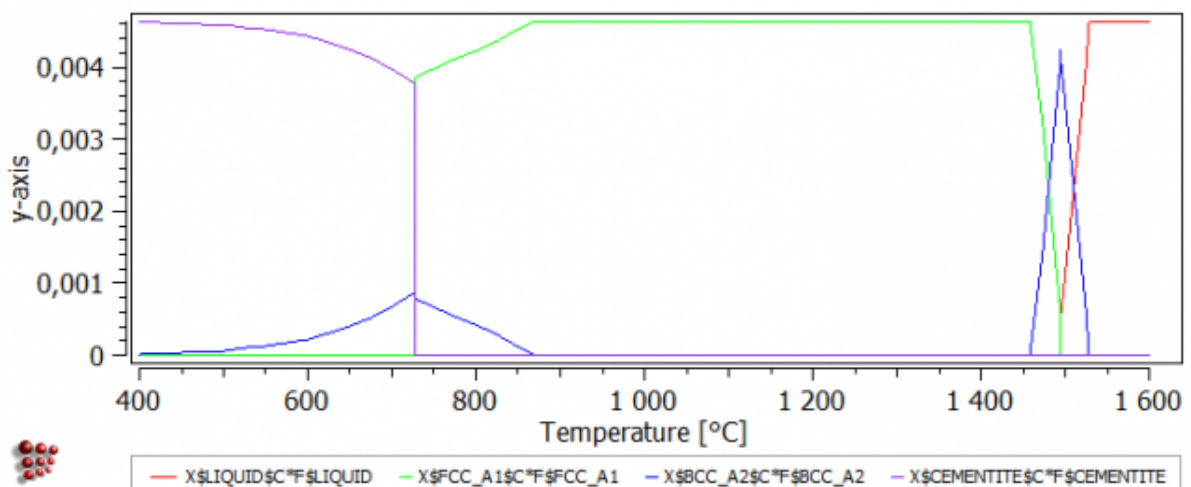
The phase fraction '**F\$***' represents the number of moles of phase per mole of system, and the carbon content of a phase '**X\$*C**' represents the number of moles of carbon per mole of phase. The product of these quantities for a given phase gives the number of moles of carbon in the phase.

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\$LIQUIDC**'. 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: '**X\$S\$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:

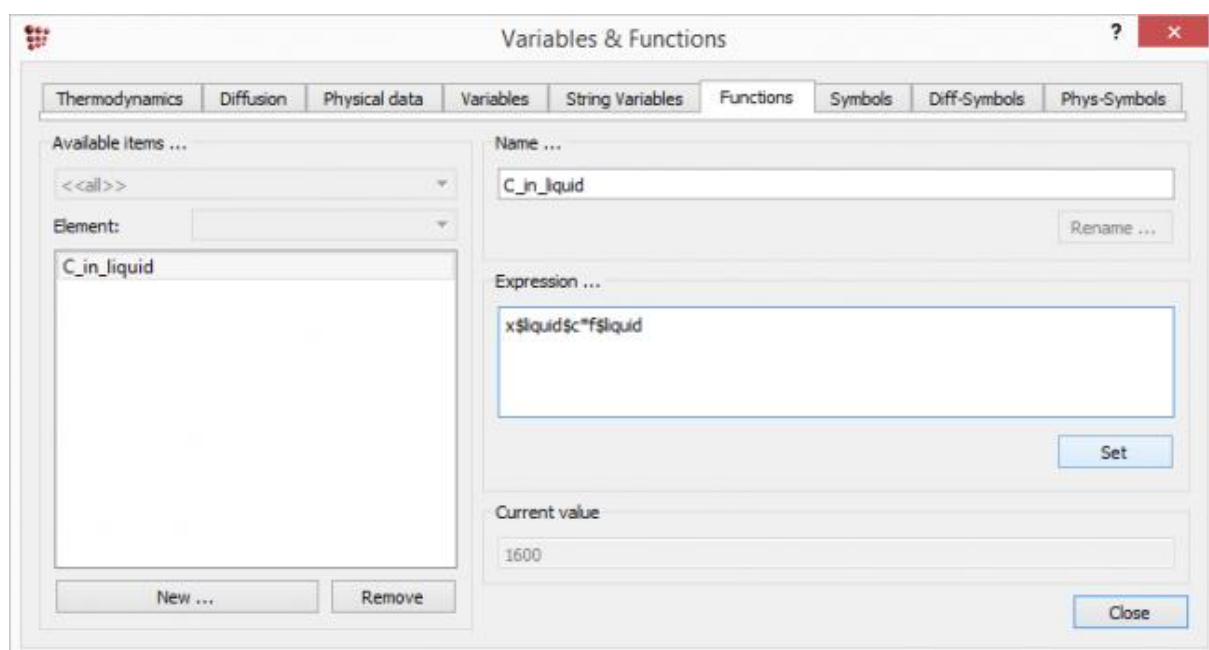


DEFINING FUNCTIONS

CREATING A NEW FUNCTION

If the expressions such as ' $X_{\text{BCC}_2} \cdot F_{\text{BCC}_2}$ ' 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 ' $x_{\text{liquid}} \cdot f_{\text{liquid}}$ '. 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:

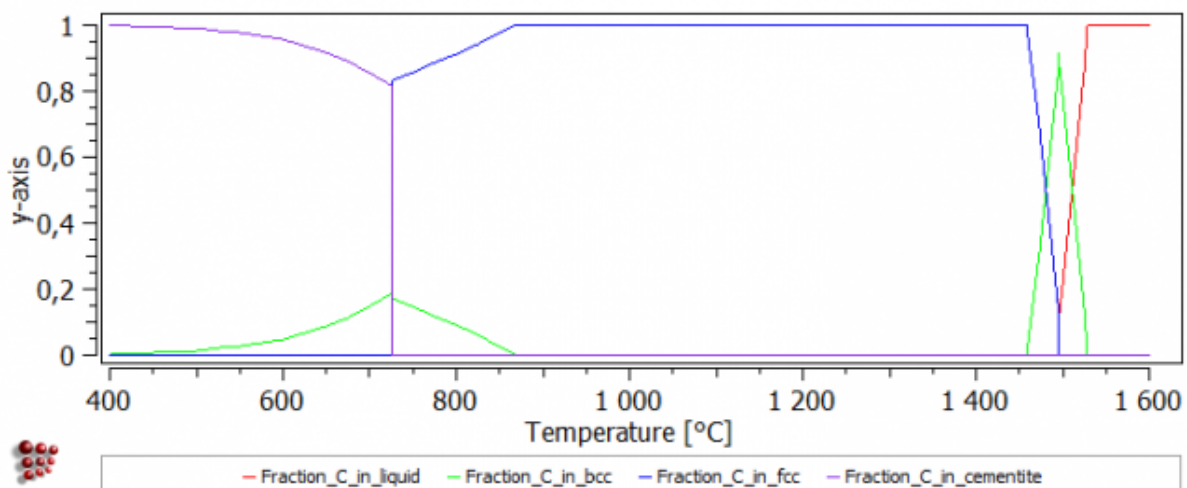
variables	value
▷ favorites	
▷ variables	
▣ functions	
C _{in_liquid}	0
C _{in_bcc}	0
C _{in_fcc}	0.00463275
C _{in_cementite}	0
▷ general	

Make a new plot and drag and drop the functions just defined into it (To select multiple entries, hold '**Ctrl**'-key while clicking on them), 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**' tab in '**Variables & Functions**' window 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.

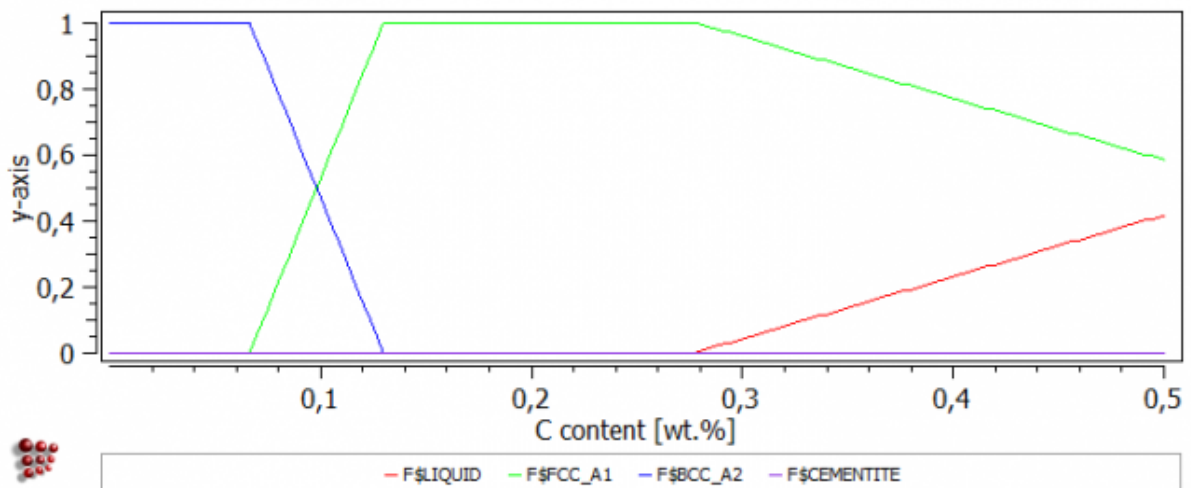
On returning to the main screen, create a new plot and drag and drop the new '**Fraction_C_in...**' functions into it. (This may necessitate clicking on the triangle sign by the side of '**Functions**' to close and re-open it with the new functions displayed.) The resulting plot should have the same appearance as the two plots above, but a different y-scale, this time going from 0 to 1.



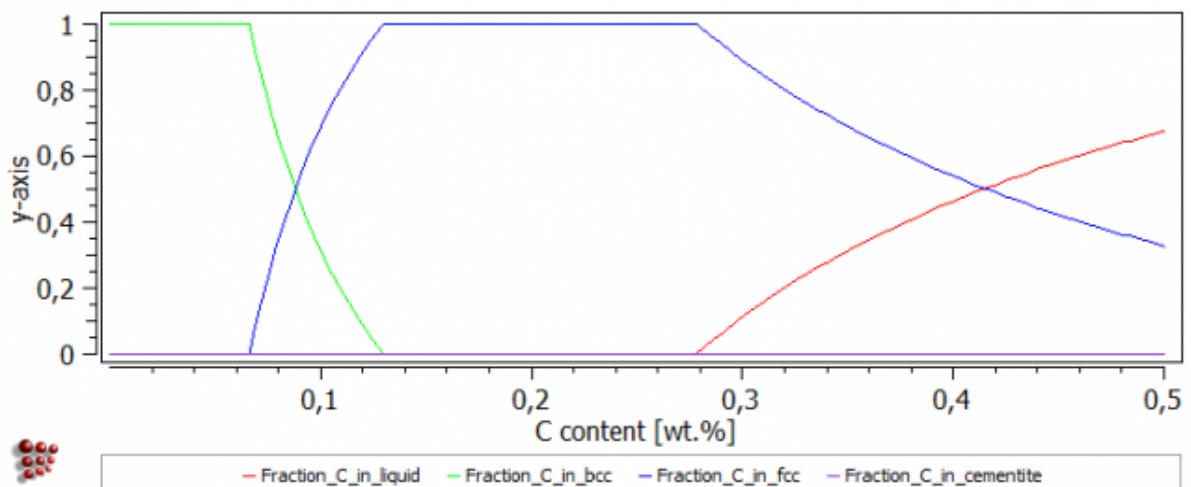
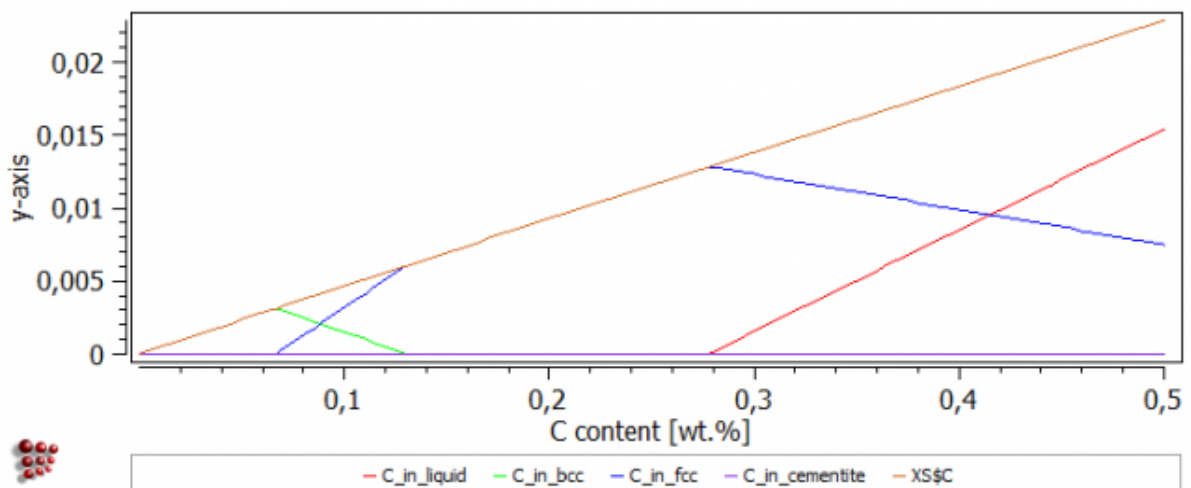
The user-defined functions are saved in the workspace and can be used for all subsequent calculations in that workspace.

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'**.

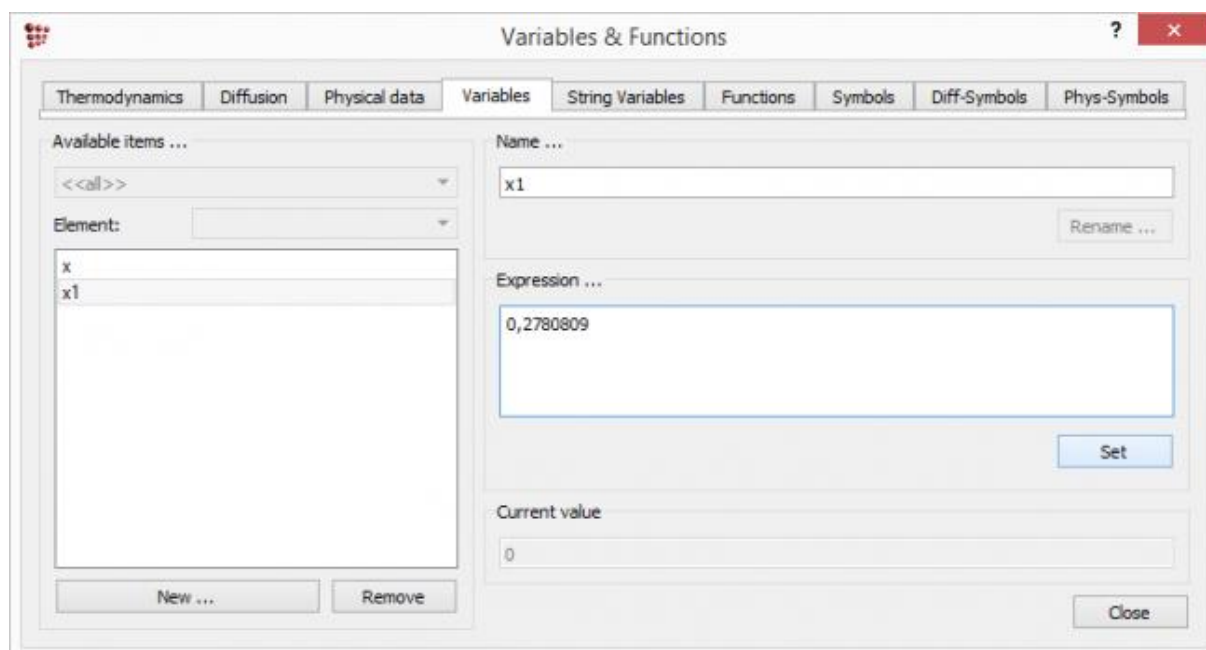
In the plot of C_{in_liquid} , C_{in_bcc} , etc., the curves are made up of almost straight-line sections, so it should be possible to find analytical expressions of the form $y = ax + b$ for these, where **'a'** is the gradient and **'b'** the intercept on the y-axis.

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 **'console'** 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 (i.e. '0.2780809') in the **'Expression'** box (confirmed by clicking on **'Set'**).



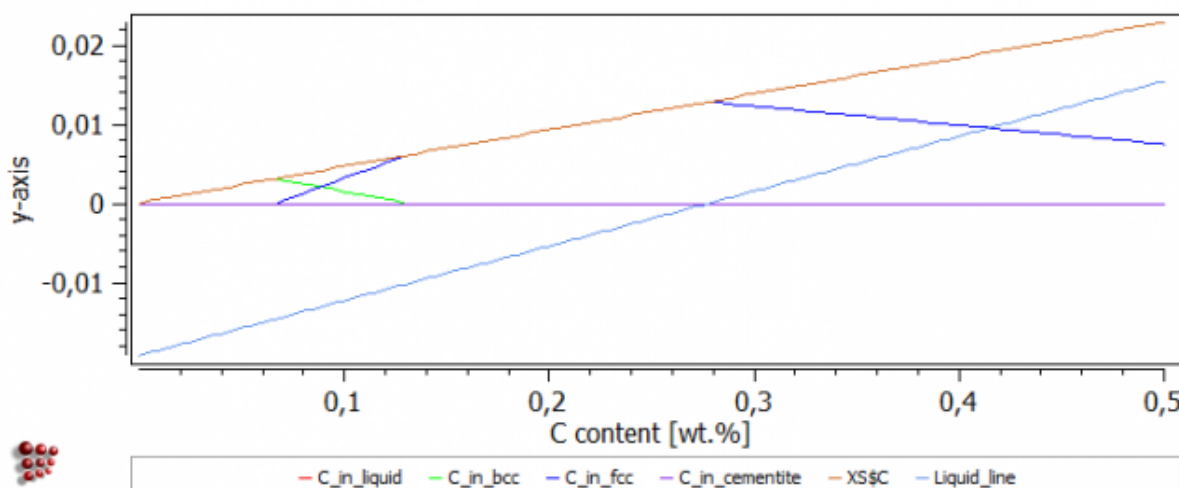
Add another variable '**y1**'. This has a default value of zero, which does not need to be changed. The second (x, y) pair can be obtained by finding the y-value at x=0.5. Either use edit the buffer state for this composition ('**Global > Buffers > Edit buffer state**', click on '**0,5**' in the '**Buffer**' 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 'Functions&Variables' window and add the new variables '**x2**' and '**y2**', equal to 0.5 and 1.536688764453e-002 in the 'Variables' tab, respectively.

The slope **a** and intercept **b** of the straight line can now be entered; **a** is equal to $(y_2 - y_1) / (x_2 - x_1)$ and **b** to $((x_2 * y_1) - (x_1 * y_2)) / (x_2 - x_1)$. 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.

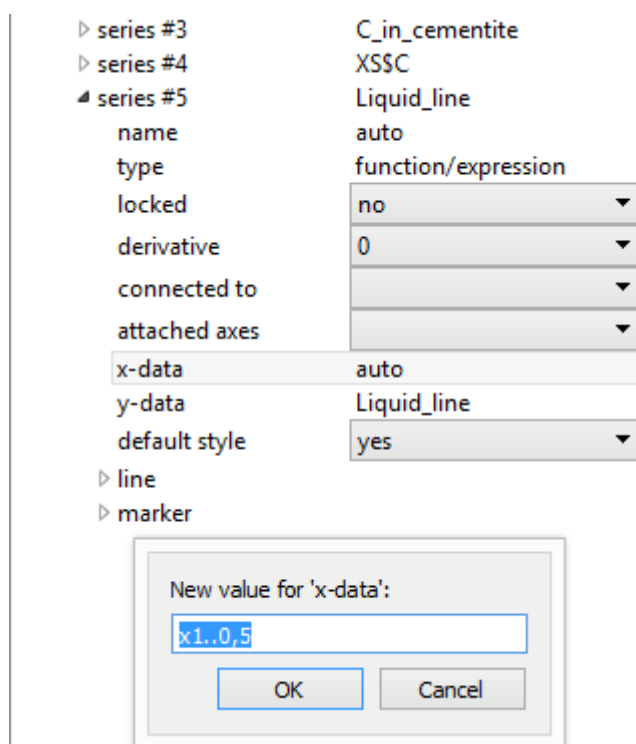
Drag the new '**Liquid_line**' function from the '**Variables**' window to the plot of '**C_in_liquid**', etc. The resulting plot should look like this:



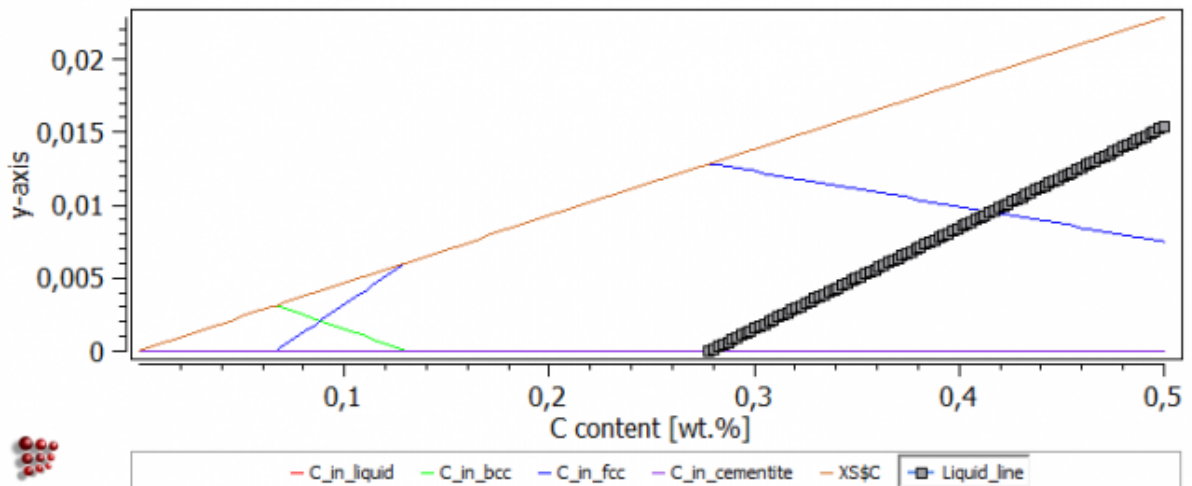
The '**Liquid_line**' function extends to negative values, unlike the true C_in_liquid curve, which has a value of zero for carbon contents between zero and 0.27 wt.%.

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).



T7: CALCULATING PHASE BOUNDARIES

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

database: mc_fe.tdb

CONTENTS

- Using “Search phase boundary” with temperature variation to determine solidus and liquidus
- Determining austenite \leftrightarrow 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 with the name '**FCC_A1#01**' has automatically been created, and examination of its composition shows that its approximate formula is NbC.

```
#### /FCC_A1/ moles: 0,996502, gm: -62325,1 (-62325,1), sff: 0,997076
Phasestatus: entered - active
FE +9,97050e-001   C +2,92362e-003   NB +2,62293e-005

#### /FCC_A1#01/ moles: 0,00349802, gm: -114284 (-114284), sff: 0,506896
Phasestatus: entered - active
NB +5,06795e-001   C +4,93104e-001   FE +1,00596e-004

### inactive ###

#### /BCC_A2/ moles: 0, gm: -62254,4 (-62254,4), sff: 0,999712
Phasestatus: entered - not active (dfm=-81,754)
FE +9,99657e-001   C +2,87522e-004   NB +5,51948e-005

#### /LIQUID/ moles: 0, gm: -58550,3 (-58550,3), sff: 1
Phasestatus: entered - not active (dfm=-3790,2)
FE +9,76688e-001   C +2,25713e-002   NB +7,40511e-004

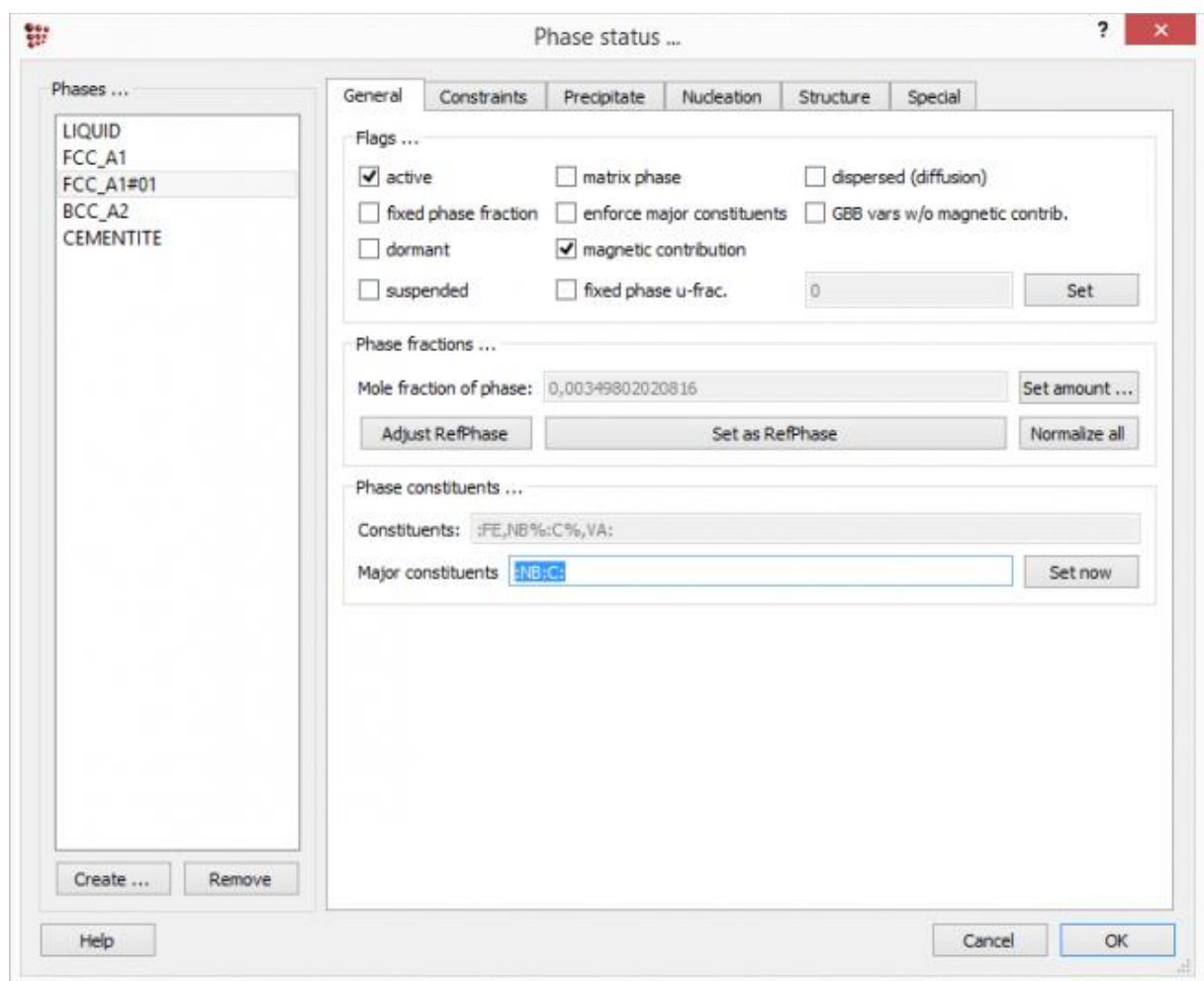
#### /CEMENTITE/ moles: 0, gm: -52498,1 (41843,9), sff: 0,25
Phasestatus: entered - not active (dfm=-9166,8)
```

```
FE +7,49088e-001  C +2,50000e-001  NB +9,11980e-004
```


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

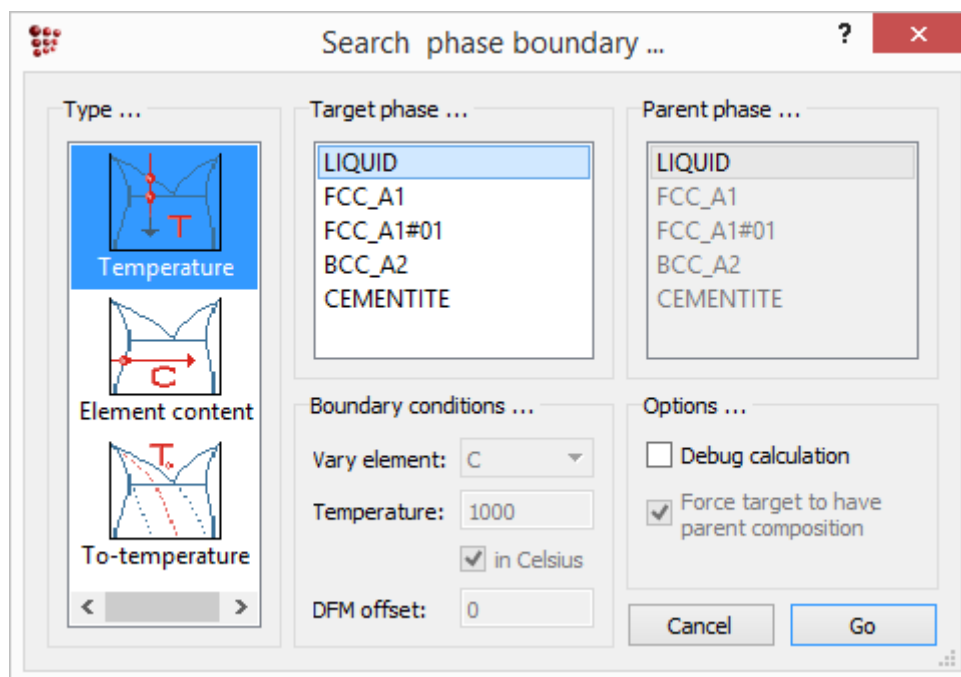
```
ADD_COMPOSITION_SET FCC_A1 :TI,NB,V:C,N: !
```

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.



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 console window.

```
Tsol 'LIQUID': 1478,08 C (1751,24 K) iter: 15, time used: 0,03 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': 1433,30 C (1706,46 K) iter: 13, time used: 0,01 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 was 1478.08°C in this case (the liquidus temperature). Information given in **'Phase summary'** window explains that at 1433.30°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 equilibrium 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': 1527,57 C (1800,73 K) iter: 4, time used: 0,02 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 phase boundary of 'BCC_A2') 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': 726.52 C (999.68 K) iter: 5, time used: 0.03 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': 883,61 C (1156,77 K) iter: 5, time used: 0,01 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.

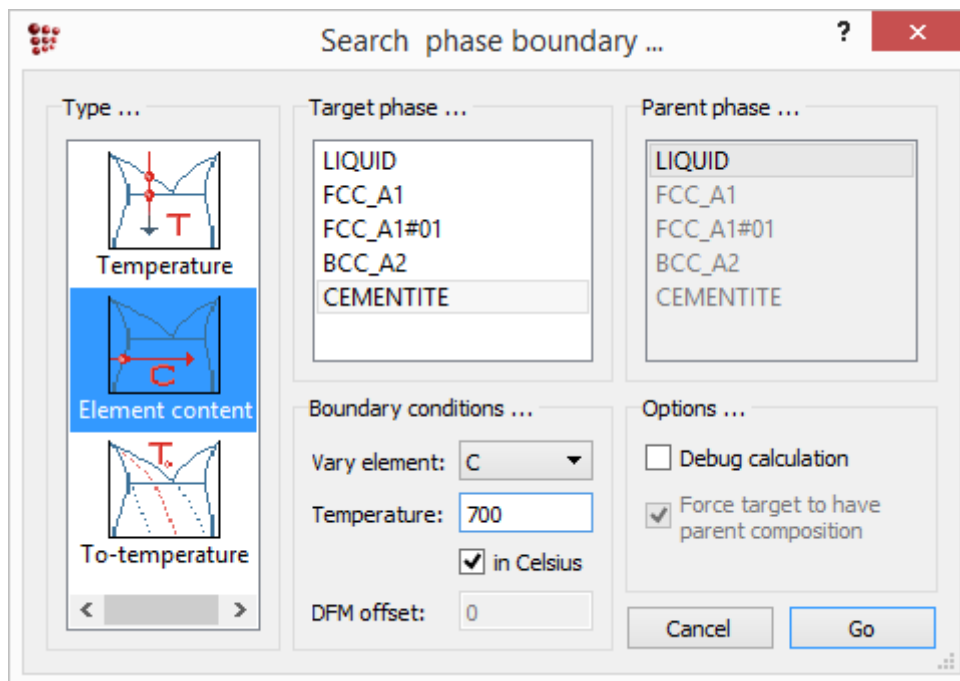
```
Tsol 'CEMENTITE': 726,52 C (999,68 K) iter: 9, time used: 0,02 s
```

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 1500°C before searching for the boundary.

```
Tsol 'FCC_A1#01': 1434,69 C (1707,85 K) iter: 16, time used: 0,03 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**'.

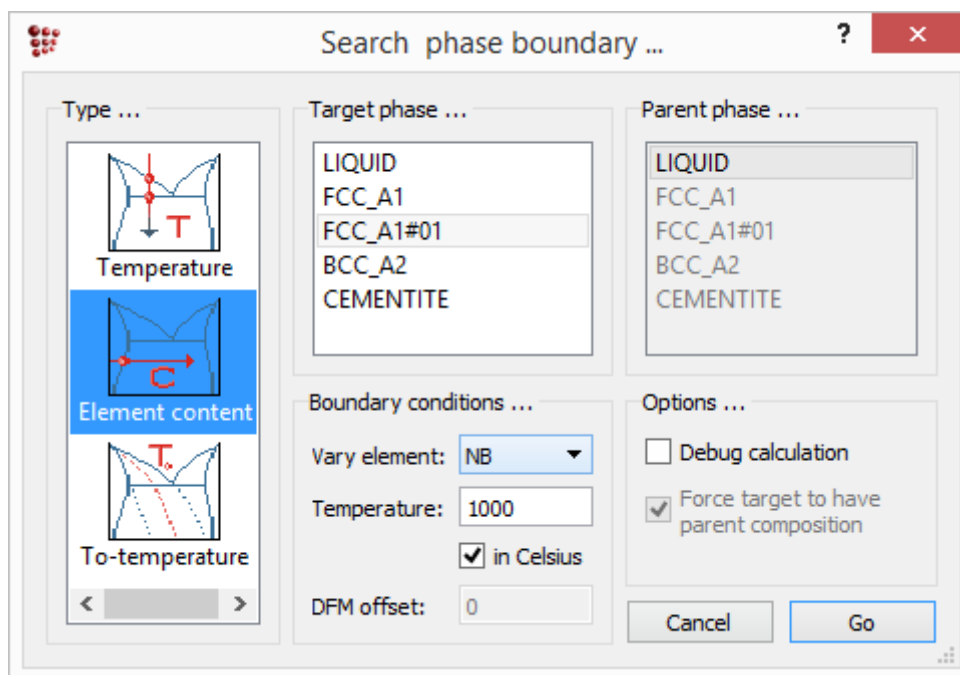


The output gives the carbon content for zero phase fraction of cementite in mole fraction and in weight percent.

```
iter: 2, time used: 0,03 s, GibbsEnergy: -40690,502 J
X(C): 0,0024754648, WP(C): 0,053279574, 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**'.



The output in the console shows the Nb content above which the carbide phase is thermodynamically stable.

```
iter: 7, time used: 0,02 s, GibbsEnergy: -62314,291 J
X(NB): 1,7315076e-005, WP(NB): 0,002890995, 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 carbide 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**', '**0.35**' and '**0.01**' as the start, stop and step interval values in the '**Range**' box. Click on '**Go**' to perform the calculation.

Step equilibrium ...

Type ...

- Temperature
- Element content
- To-temperature
- Phase boundary**
- Defect density

Range ...

Start: 0,01
 Stop: 0,35
 Step interval: ☒ linear ☐ logarithmic

☐ vary T only, do not evaluate equilibrium

Options ...

☒ Temperatures in Celsius
☒ Composition in weight percent
☐ Append
☐ Append w/o load
☐ Reverse sort order
☐ Automatically save
☐ Force identical composition

vary ...

☒ global comp. ☐ paraequ. u-constr.

Boundary conditions ...

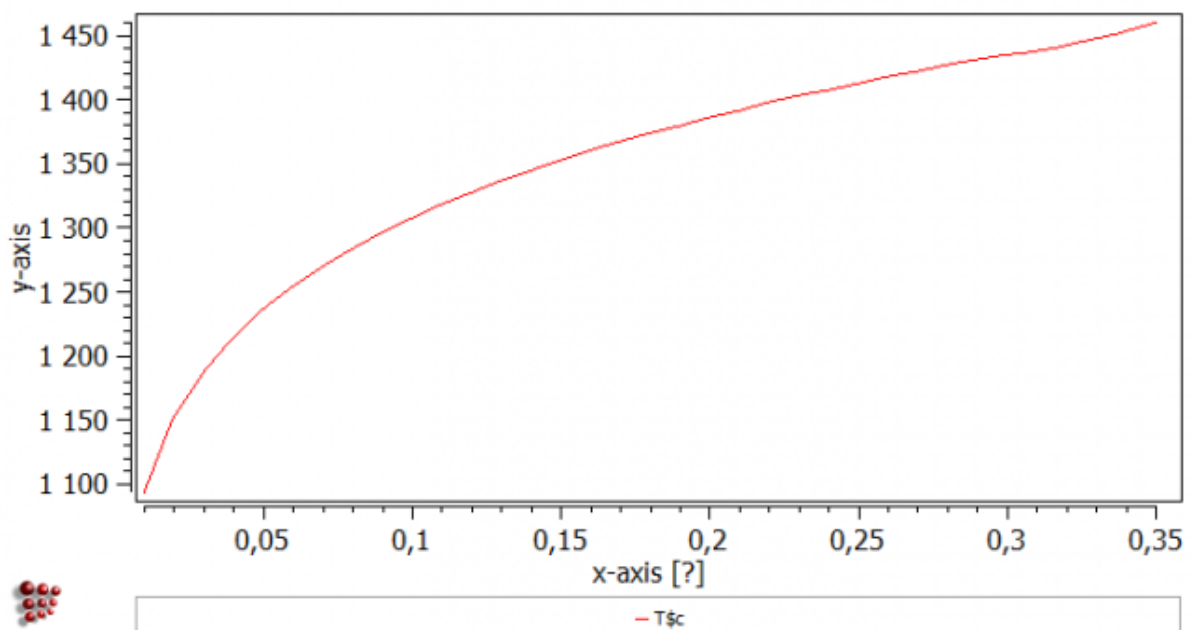
element: NB
 temperature C: 1000
 Target phase: FCC_A1#01
 Parent phase: LIQUID
 max. T-step: 100
 dfm-offset: 0

Impose transformations ...

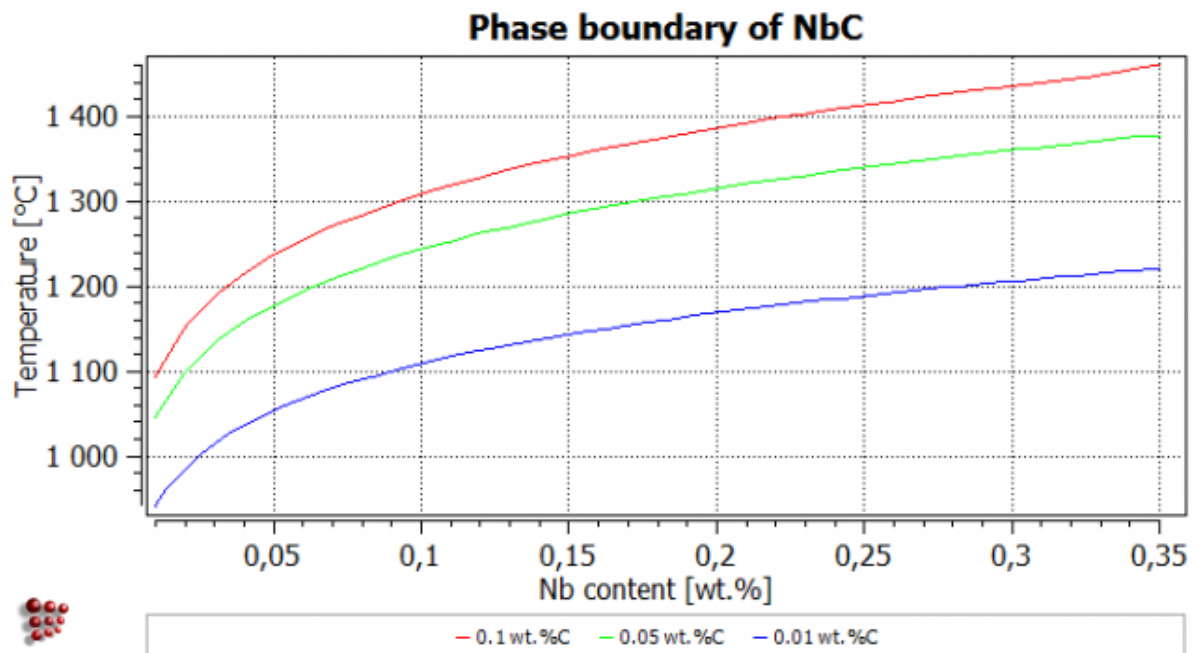
Add ... Remove Edit ...

Cancel Go

Create a new X-Y plot window (Tutorial 4) and drag and drop '**T_{sc}**' (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 - as an exercise you can try to format the plot as shown below.



T8: CALCULATING A PHASE DIAGRAM IN A BINARY SYSTEM

***This tutorial was tested on
MatCalc version 6.00 rel 0.100
license: free
database: mc_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

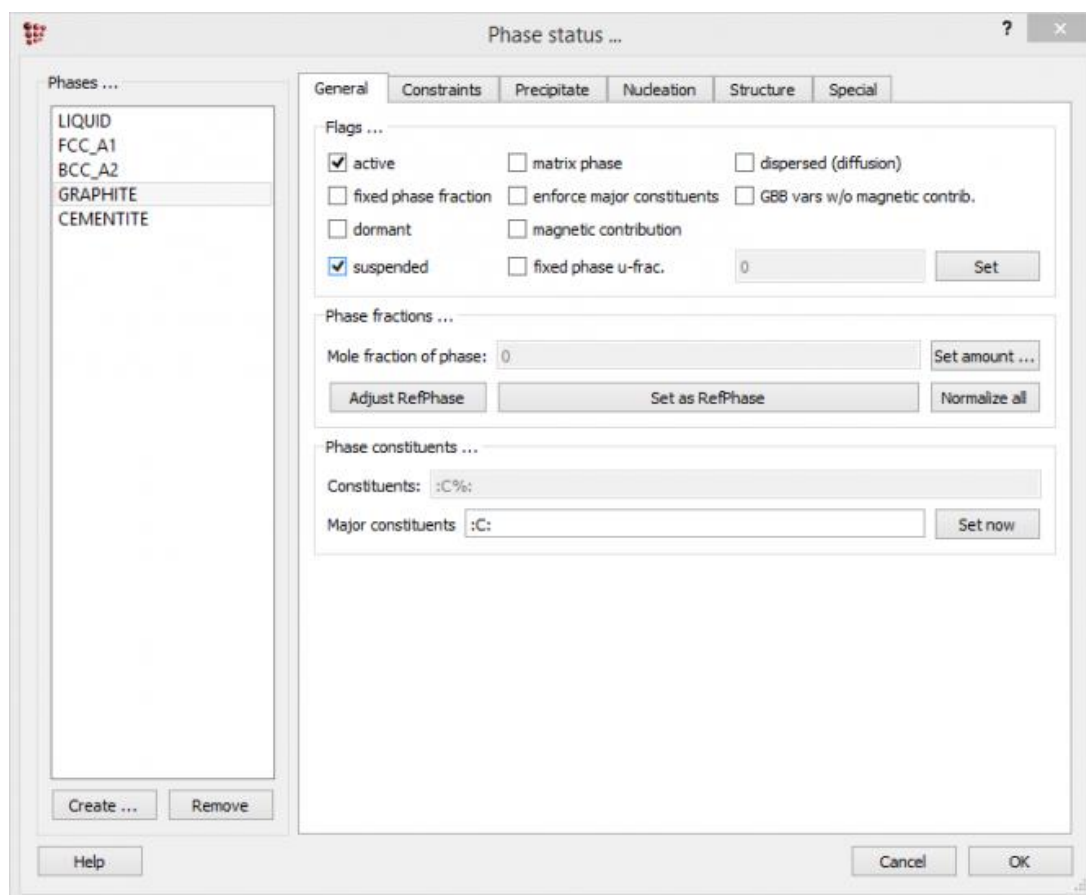
A phase diagram consists of a number of phase-boundaries separating regions of temperature- and composition-space in which different phases are stable at equilibrium. Published equilibrium diagrams for the Fe-C system often show equilibria between Fe-rich phases and both C (in the form of graphite) and 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_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**':





FE-Fe₃C PHASE DIAGRAM

The phase diagram is made up of a number of phase boundaries. As we 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

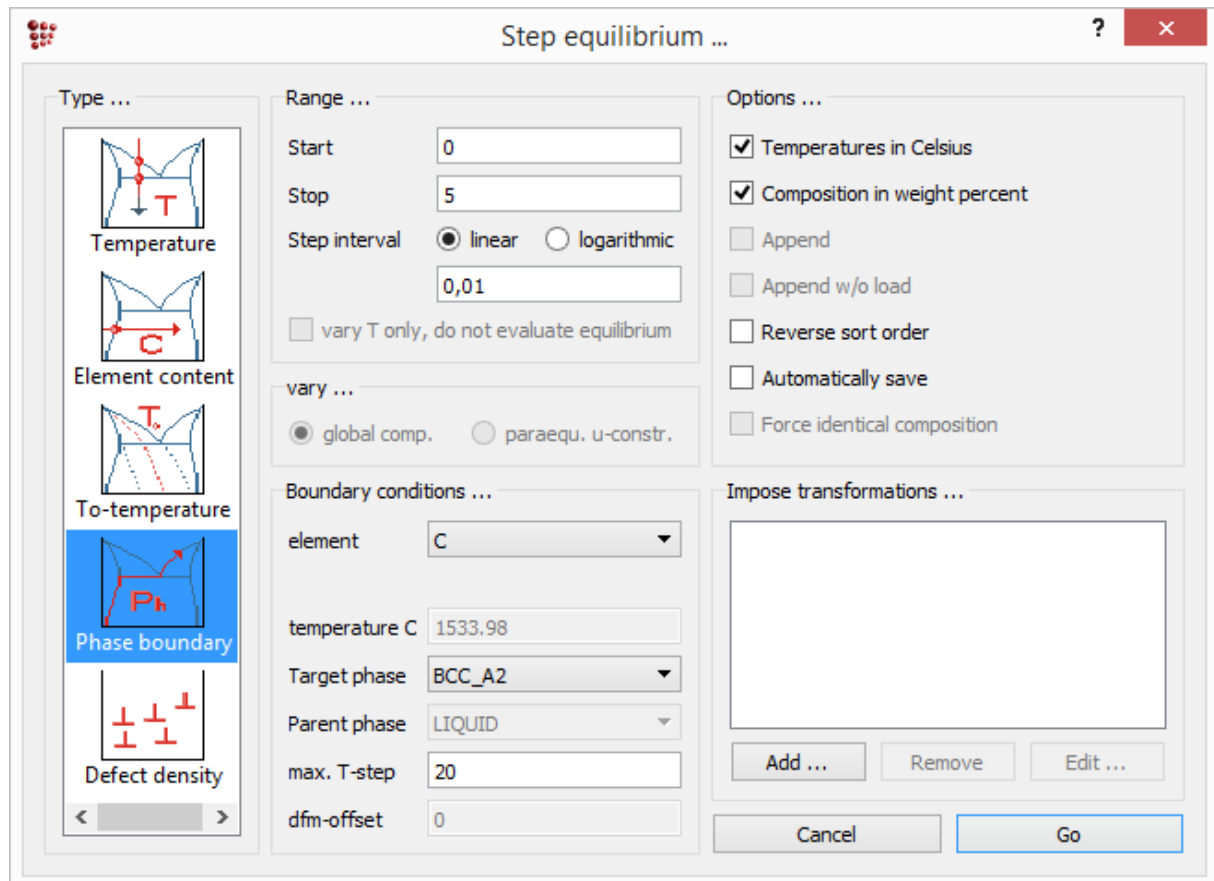
UPPER BOUNDARY OF DELTA-FERRITE, BCC_A2

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.

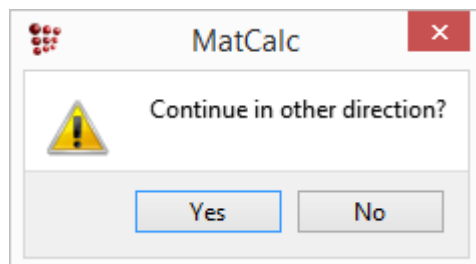
To locate the boundary, an equilibrium must first be calculated reasonably close to the expected boundary temperature. It can be seen that the line lies somewhere between 1538°C (the melting temperature of pure iron) and 1500°C. Click on the  icon and enter the temperature '1530'. (If this gives an error 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: 8, time used: 0.03 s
```

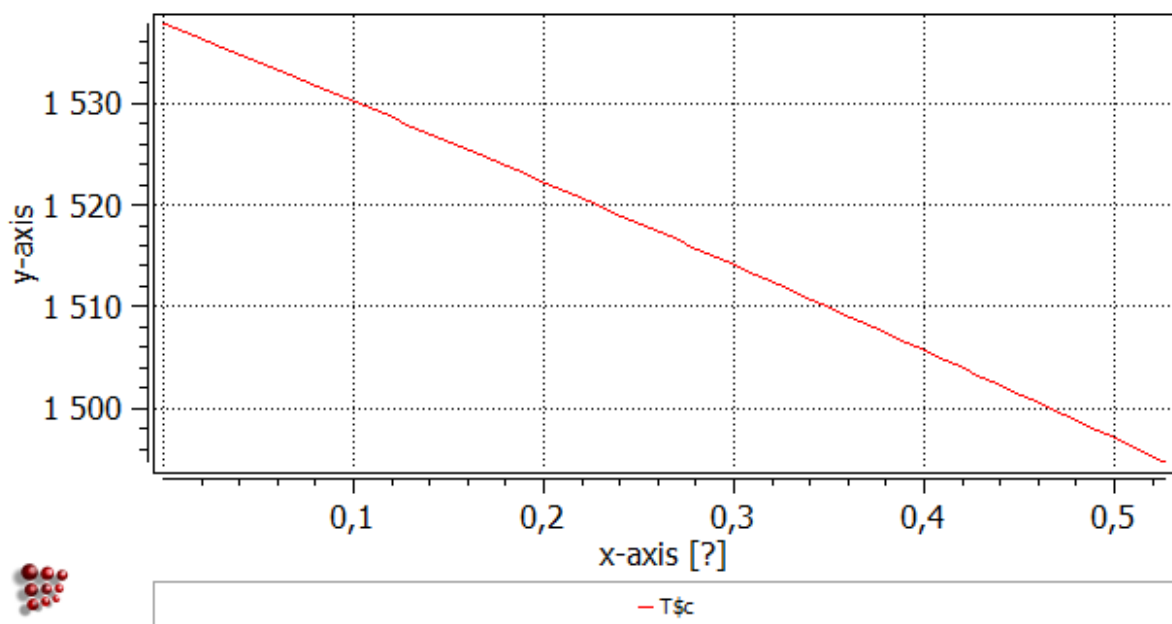
This shows that a point on the boundary has been found successfully. The next step is to trace this boundary using the stepped equilibrium function to vary the carbon content. Click on  and choose '**Phase boundary**' from the left-hand column. Enter the range: '0' to '5', in intervals of '0.01'. Select '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 (With plot window selected, go to 'Options' window and in 'plots'>'plot#0'>'grid' select 'enabled' for 'major-x' and 'major-y'). 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.



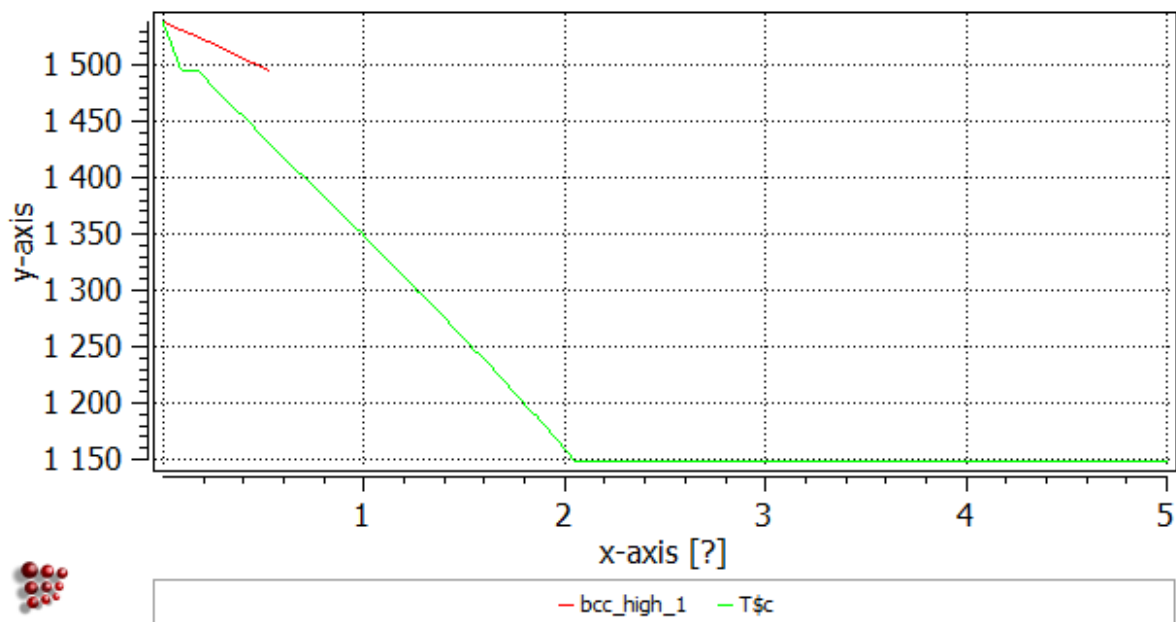
Right-click in the plot window outside the plot area itself, and select '**Duplicate and lock series**' from the menu displayed. Select the name of the series and click '**Duplicate**' to produce a copy of the series. In the '**options**' window, rename the first series '**bcc_high_1**'.

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: 0.03 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-12**' to facilitate the calculation.) The diagram should now look like this:



Don't forget to duplicate and lock this new series!

LOWER BOUNDARY OF DELTA-FERRITE (BCC_A2)

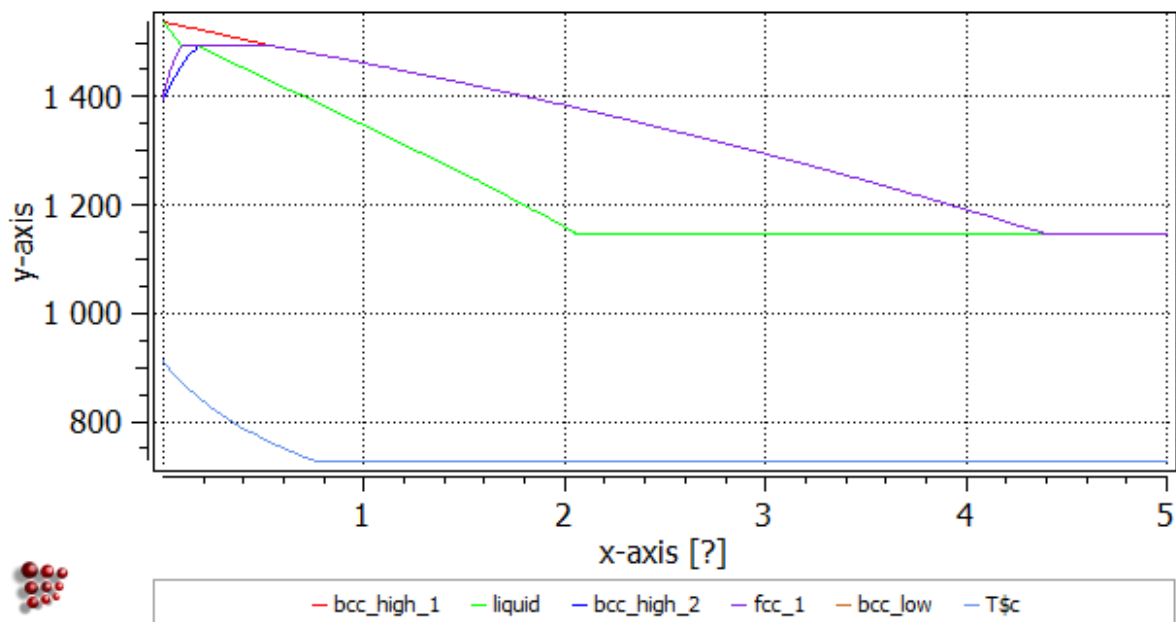
Calculate an equilibrium at 1400°C, search for BCC_A2 (the boundary temperature should be 1429.60 C (1702.76 K)), step from 0 to 5 wt.% C with an interval of 0.01 wt.% C. Accept the **'Continue in other direction'** message (the calculation could not reach 5 wt.% C limit, again) with **'Yes'**.

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.

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 726.52°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 726.52°C. Using the same settings as for the previous stepped calculation, the phase boundary is calculated correctly, but might extend 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-12, 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

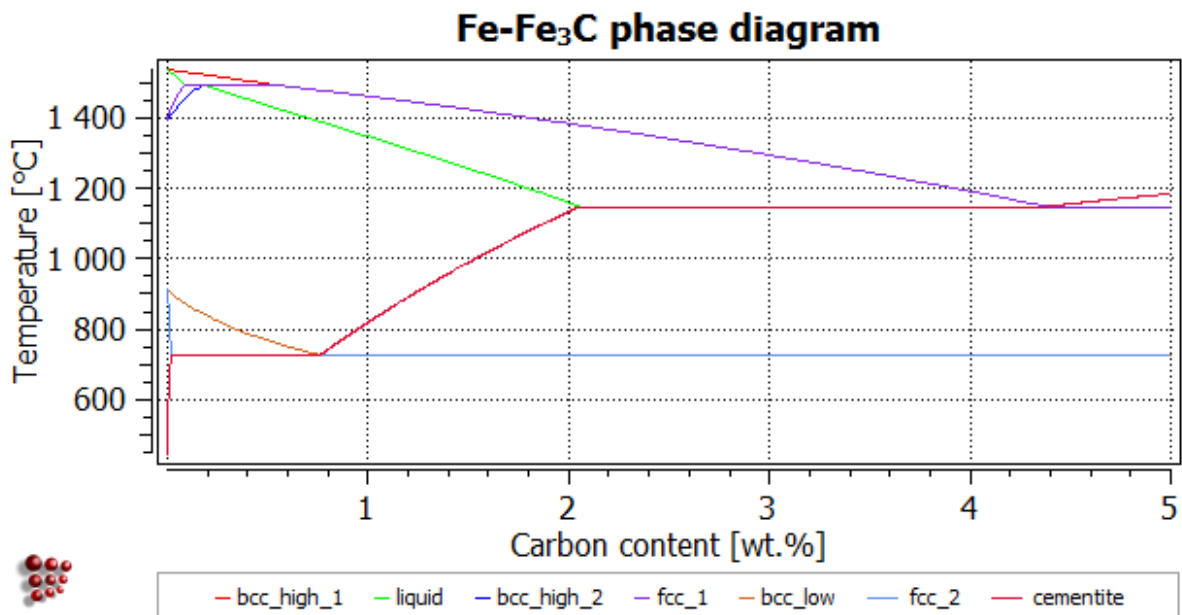
Following a phase boundary in the stepped calculation is performed by a simple procedure. Once an initial point is found with '**Search phase boundary**' operation, the composition of the system is changed by a value specified as a step in the '**Range**' section of '**Stepped equilibrium**' window. 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 equilibrium phases (due to the undefined chemical potentials for these phases)

THE FINISHED DIAGRAM

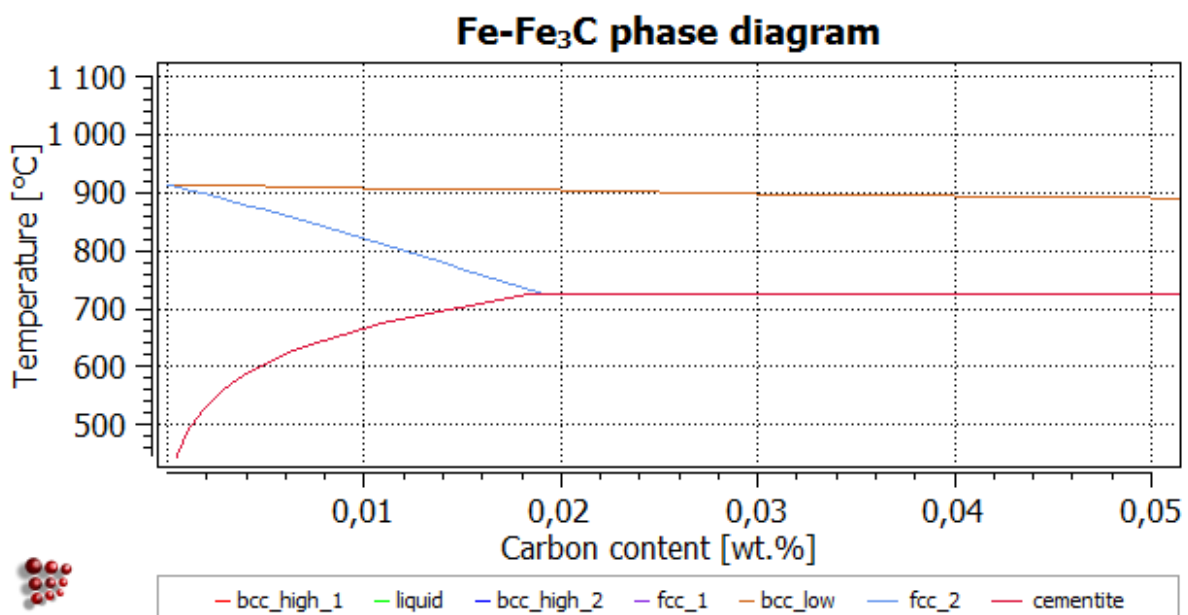
Do not forget to lock the last series to be added, so that it is not modified when another calculation is performed. Add axis labels and a title '**Fe-Fe₃C phase diagram**'. The subscript can be obtained using HTML tags:

```
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 presenting the phase solubility of alpha-ferrite.

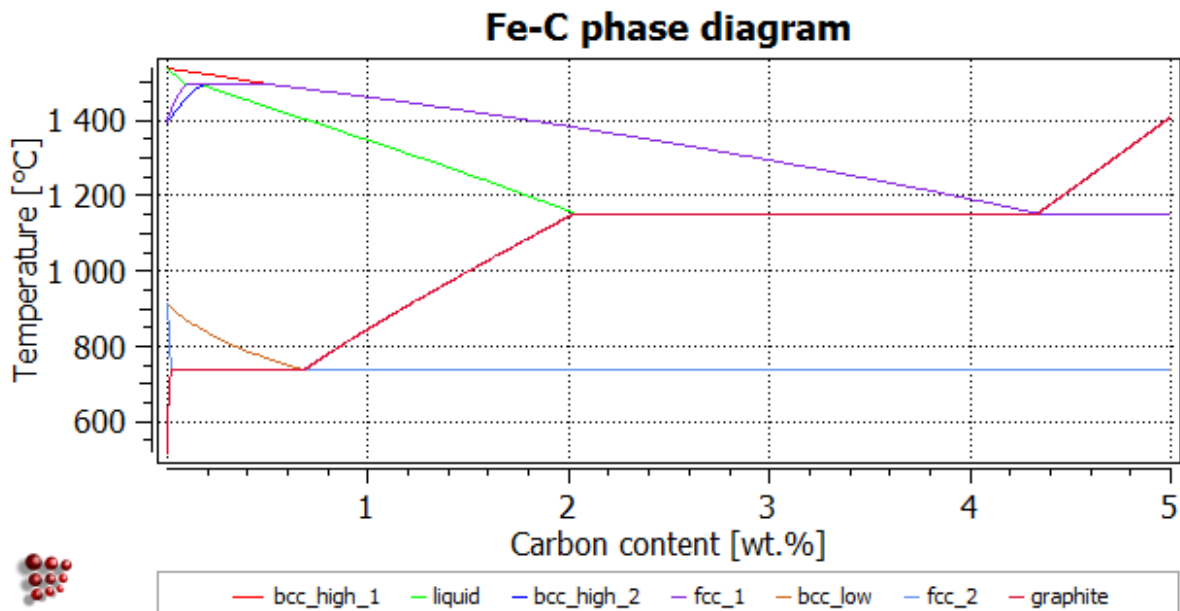


FE-C PHASE DIAGRAM

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.)



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). If problems occur, decrease the interval to 0.001 as well as increasing the T-step to 100 to obtain better resolution of the phase boundary 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-12.

T9: CALCULATING PSEUDOBINARY PHASE DIAGRAMS

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

database: mc_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

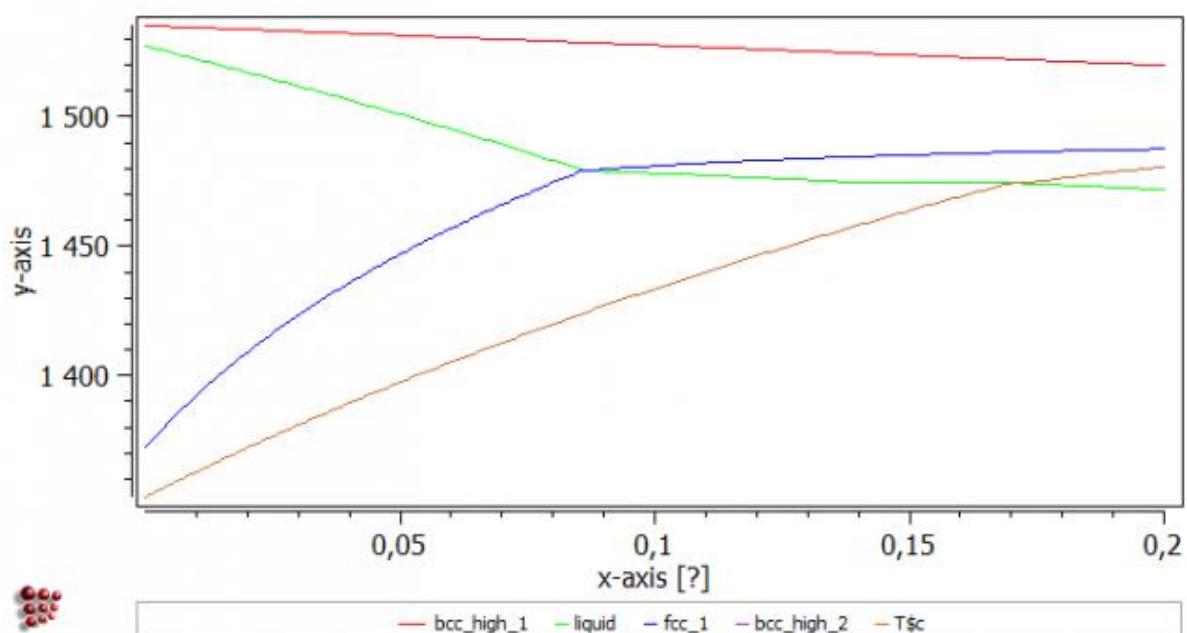
Make a new workspace with the elements Fe, C and Nb and the phases FCC_A1, BCC_A2, LIQUID and CEMENTITE. Verify that Fe is selected as the reference element and enter the composition: 0.1 wt.% C, 0.3 wt.% Nb. Create a new p1-type plot window for the phase diagram.

FE-C PSEUDOBINARY WITH CONSTANT NB CONTENT

This is similar in many respects to the Fe-Fe₃C 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 0.001 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 T_{sol} 'FCC_A1' should be 1480.93°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

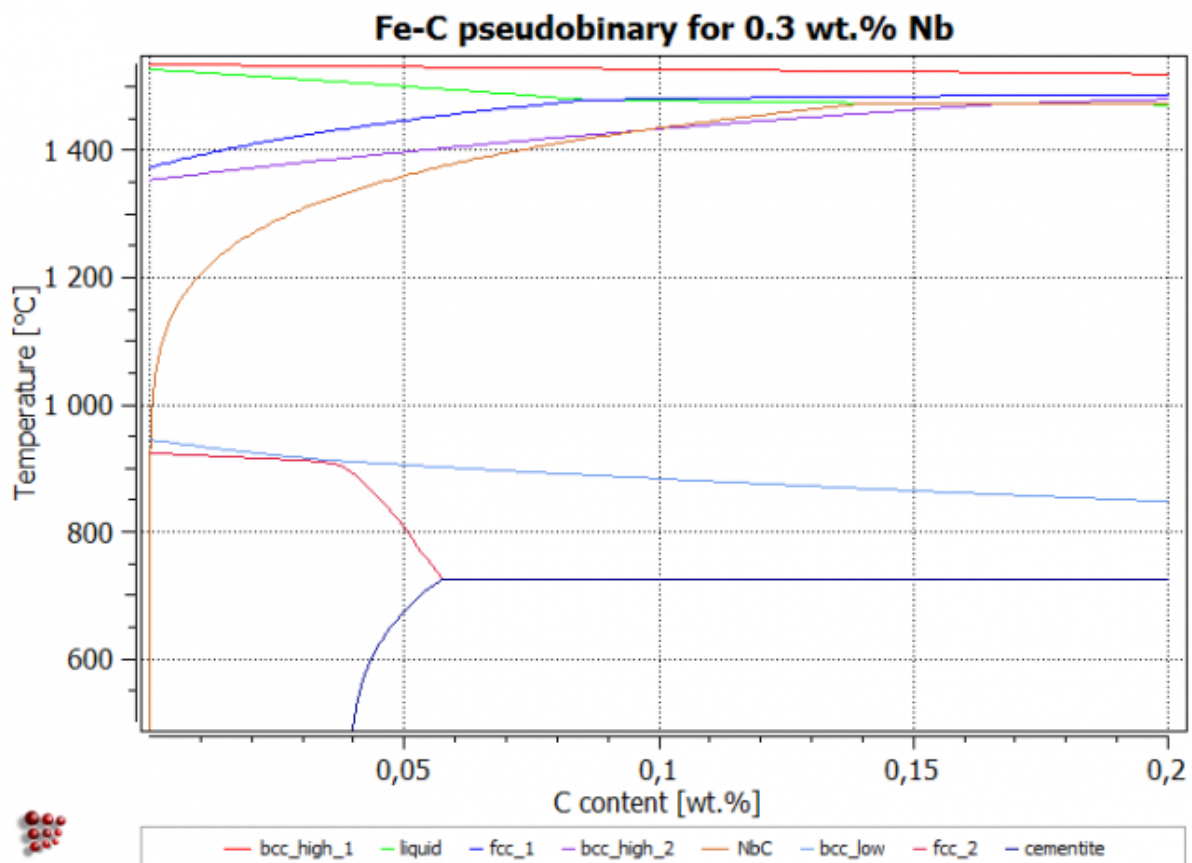
starting point for finding it.

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:



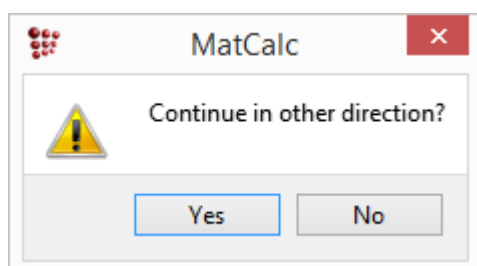
FE-NB PSEUDOBIINARY WITH CONSTANT C CONTENT

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:

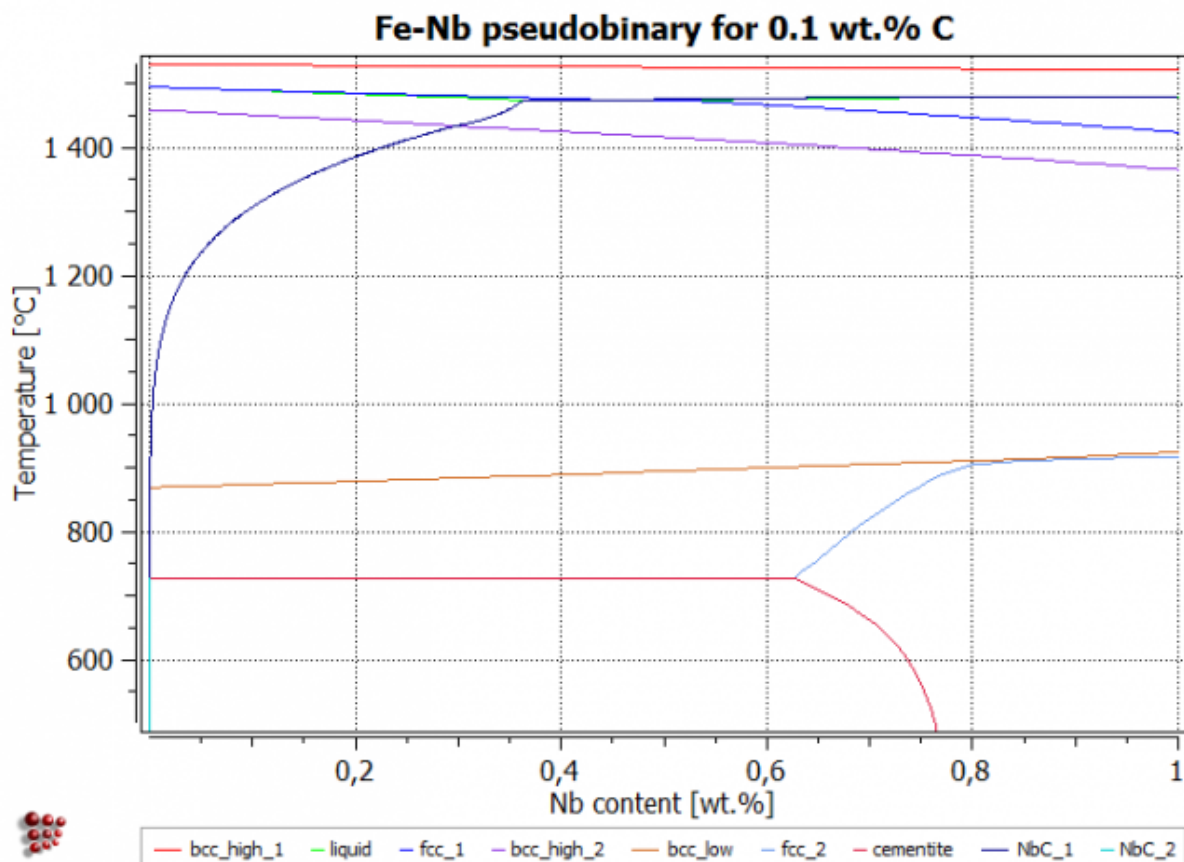
- Upper boundary of delta-ferrite (BCC_A2)
- Lower boundary of liquid
- Upper boundary of austenite (FCC_A1)
- Lower boundary of delta-ferrite
- Upper boundary of alpha-ferrite (BCC_A2)
- Lower boundary of austenite
- Upper boundary of cementite (may need modification of maximum T-step to 100-200)

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 1000°C and search for the FCC_A1#01 phase boundary varying temperature. This is at 1434.69°C. Make a stepped calculation from 0 to 1 wt.% Nb with 0,001 step and max. T-step value of 2. The calculation starts as usual 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). It can be noted, however, that the calculation terminates at the **'cementite'** line during decreasing the Nb content. In order to find the phase boundary outside these limits, additional calculations must be performed. After locking the previous curve, calculate an equilibrium at 500°C and search for the FCC_A1#01 phase boundary at this temperature (i.e. vary the Nb content). Due to the steep boundary, it is recommended to set the calculation step to 0.001 and the max. T-step value to 200. Part-way through this calculation, the following message might appear:



Just click on 'Yes' to continue the calculation.

The finished diagram is shown below.



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 by clicking in the '**Nb**' line of the '**Ref.Elem.**' column. Enter the compositions 0.996 Fe, 0.003 C.

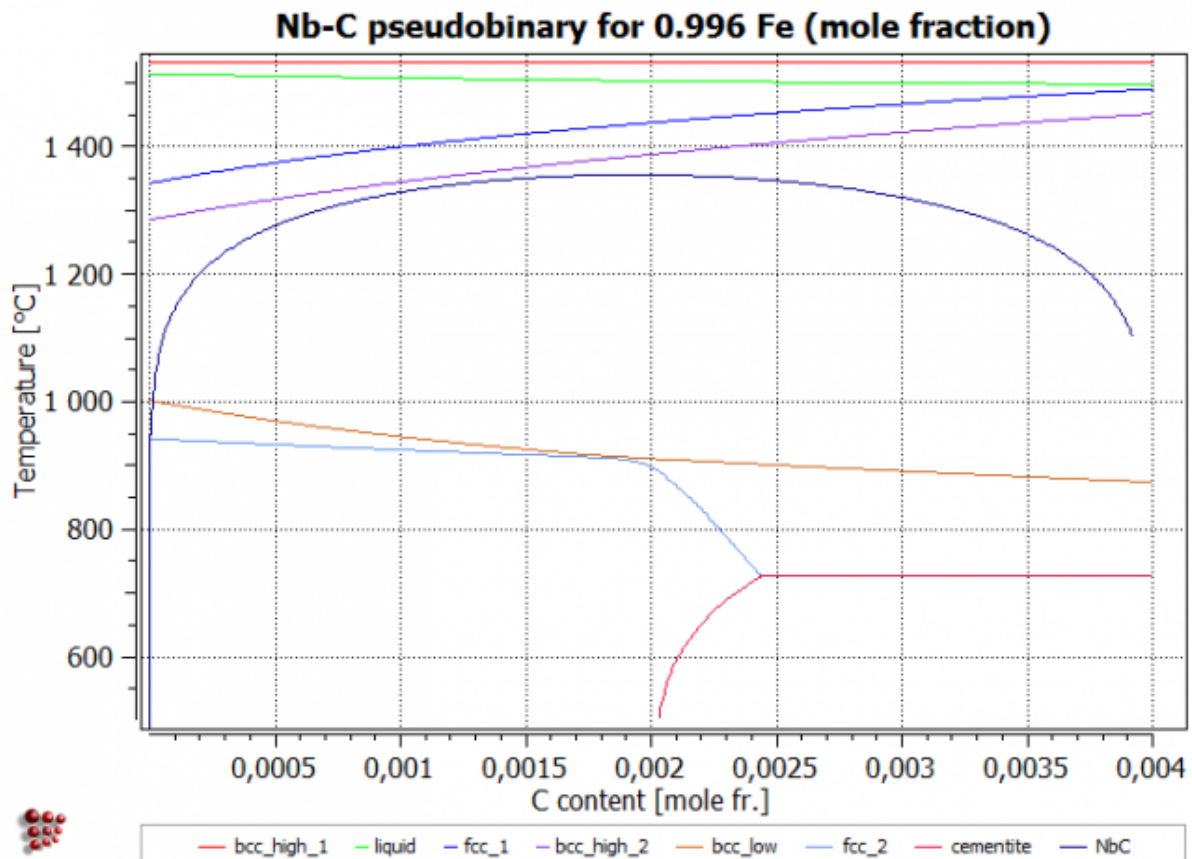
As usual, search for the upper boundary of the delta-ferrite phase. This should be found at 1531.42°C. In the stepped calculation dialogue box, enter 0, 0.004 and 1e-5 as the start, stop and interval values. Set the varying element to '**C**' and the maximum T-step to 20. In the '**Options**' section 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 (Accept any questions about changing the direction of calculation)).

- BCC_A2: 1531.42°C
- LIQUID: 1499.64°C. A warning message may appear; accept this with 'Yes'.
- FCC_A1: 1466.52°C. The same warning may appear.
- BCC_A2: 1422.52°C
- BCC_A2: 891.36°C. Step from 0 to 0.00399 rather than 0.004 to avoid convergence problems.
- FCC_A1: 726.52°C. Calculation from 0 to 0.00399 with 1e-6 step.
- CEMENTITE: 726.52°C

Finally, the line for FCC_A1#01 can be calculated. Search for this line, which should be found at 1320.29°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 0.0039 (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:



T10: T_0 -TEMPERATURE IN FE-CR-C

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

database: mc_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 **T₀-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 T₀-temperature calculations to the evaluation of transformation temperatures.

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

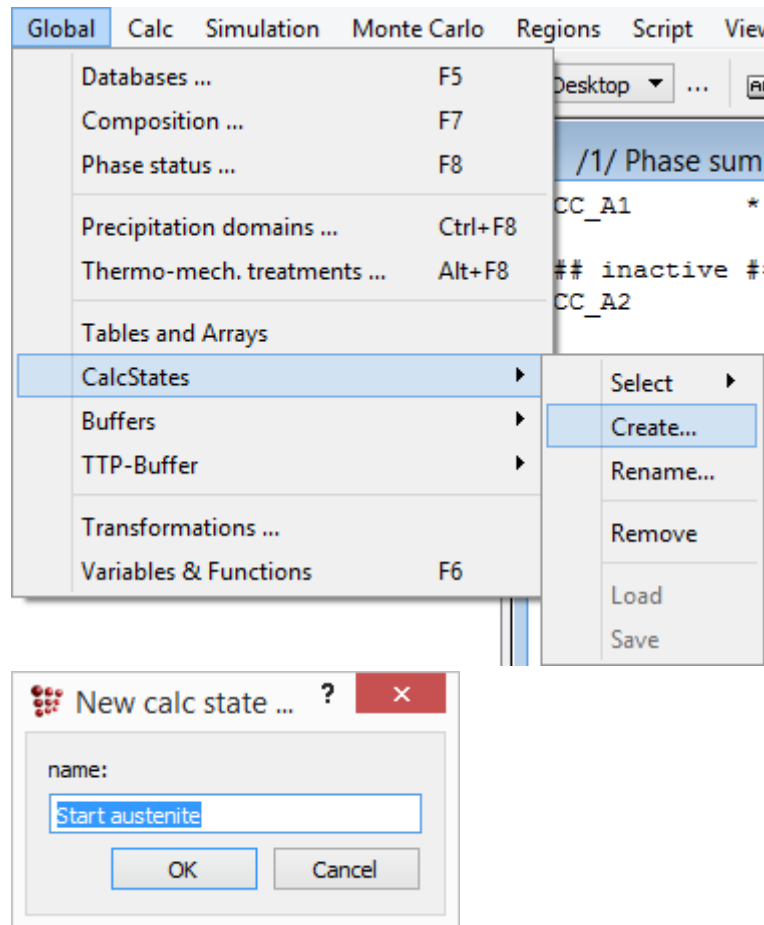
Create a new workspace file. From a suitable database (mc_sample_fe2.tdb) define the elements **Fe**, **Cr** and **C** as well as the phases **BCC_A2** (ferrite) and **FCC_A1** (austenite). Enter the system composition in weight percent with **wp(C) = 0.1** and **wp(Cr)=1.0**. Set initial values with **'Calc' → 'Set start values'** or **Ctrl+Shift+F**. Calculate an equilibrium at **800°C**.

STEP 2: CALCULATE THE T₀-TEMPERATURE

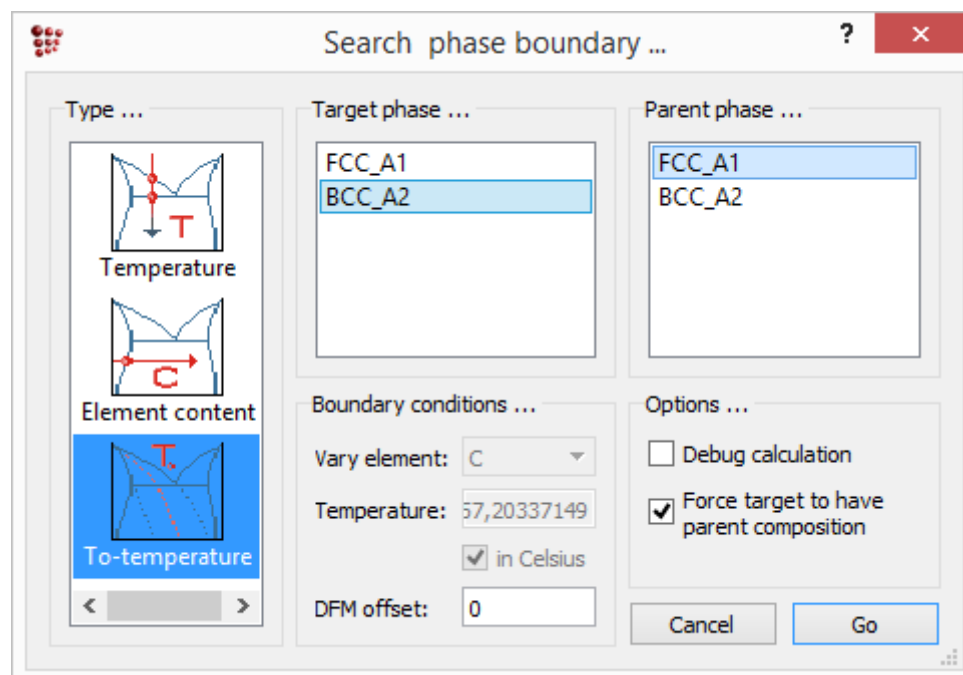
Before evaluation of the T₀-temperature, an equilibrium located in the **one-phase region** of the parent phase must be calculated in order **to set the composition of one of the phases equal to the system composition**. The parent phase is austenite so the solubility temperature of BCC_A2 will be evaluated with **'Calc' → 'Search phase boundary...'** or **Ctrl+Shift+T**. Set **'Temperature'** as type and **'BCC_A2'** as target phase, then click on 'Go'. As a result, MatCalc displays in the **'console'** window

```
Tsol 'BCC_A2': 857,20 C (1130,36 K) iter: 12, time used: 0,02 s
```

In the **'Phase summary'** and **'Phase details'** window, only the FCC_A1 phase is denoted as active (mole fraction = 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 '**T₀-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 will 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) : 791,451 C (1064,61 K)
iter: 2, time used: 0,02 s
- OK -
```

The phase details window shows:

```
#### /FCC_A1/ moles: 1, gm: -46908,9 (-46908,9)
Phasestatus: entered - active
FE +9,84677e-001 CR +1,06937e-002 C +4,62933e-003

### inactive ###

#### /BCC_A2/ moles: 0, gm: -46908,9 (-46908,9)
Phasestatus: entered - not active (dfm=2,4156e-009)
FE +9,84677e-001 CR +1,06937e-002 C +4,62933e-003
```

It is thus clear that, at the temperature of 791,451°C, FCC_A1 and BCC_A2 of the same composition have the same molar Gibbs free energy of $gm = -46908.9 \text{ J/mole}$.

STEP 3: EVALUATE T₀- TEMPERATURE AS A FUNCTION OF CHROMIUM CONTENT

Let us now investigate how the T₀- 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 '**T₀ 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.

Step equilibrium ...

Type ...

Temperature

Element content

To-temperature

Phase boundary

Defect density

Range ...

Start: 0

Stop: 10

Step interval: ☒ linear ☐ logarithmic

0,5

☐ vary T only, do not evaluate equilibrium

vary ...

☒ global comp. ☐ paraeq. u-constr.

Boundary conditions ...

element: CR

temperature C: 791.45

Target phase: BCC_A2

Parent phase: FCC_A1

max. T-step: 20

dfm-offset: 0

Options ...

☒ Temperatures in Celsius

☒ Composition in weight percent

☐ Append

☐ Append w/o load

☐ Reverse sort order

☐ Automatically save

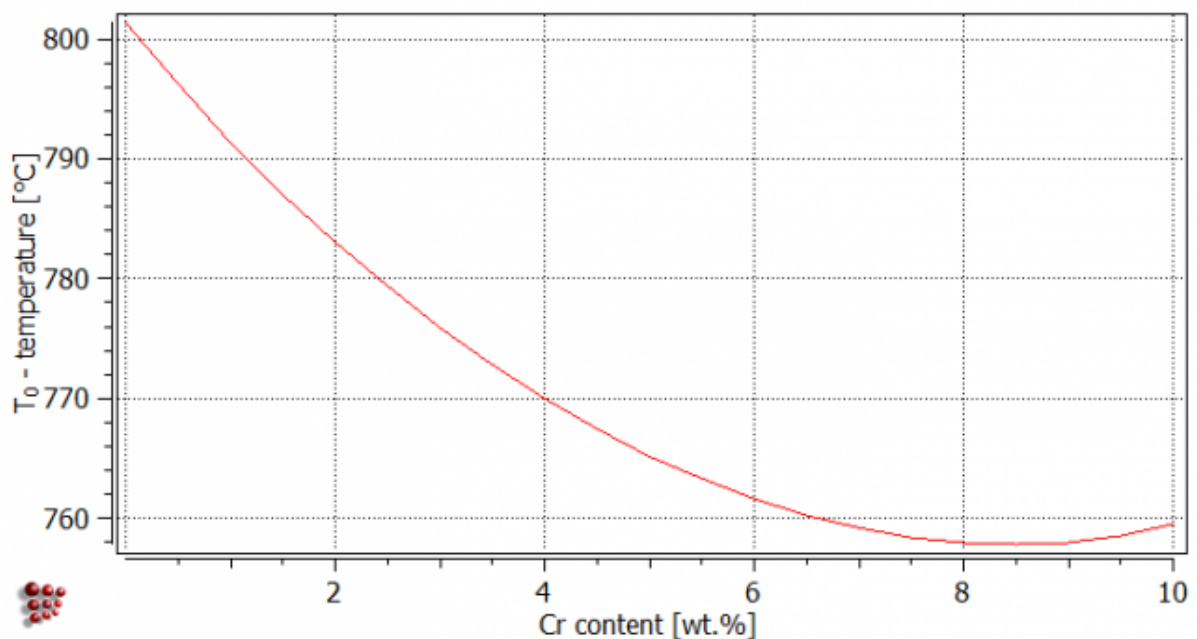
☒ Force identical composition

Impose transformations ...

Add ... Remove Edit ...

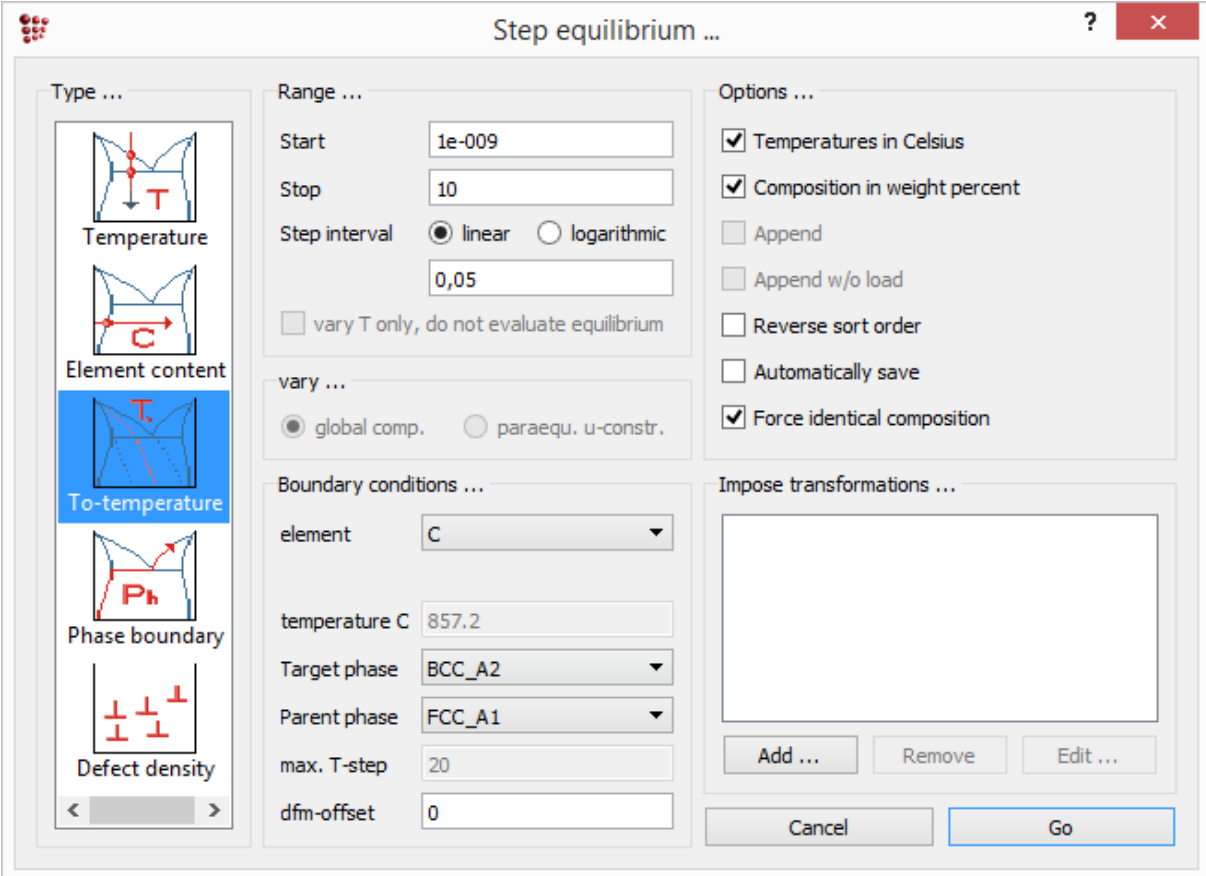
Cancel Go

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 **T₀** 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 T₀- 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 '**T0-chromium**'. Then create a new buffer ('**Global**' → '**Buffers**' → '**Create...**') with the name '**T0-carbon**' and load the calculation state '**Start austenite**' (make sure that the current buffer is the '**T0-carbon**'). 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**'.



Step equilibrium ...

Type ...

- Temperature
- Element content
- To-temperature**
- Phase boundary
- Defect density

Range ...

Start: 1e-009
 Stop: 10
 Step interval: ☒ linear ☐ logarithmic
 0,05
☐ vary T only, do not evaluate equilibrium

Options ...

☒ Temperatures in Celsius
☒ Composition in weight percent
☐ Append
☐ Append w/o load
☐ Reverse sort order
☐ Automatically save
☒ Force identical composition

Boundary conditions ...

element: C
 temperature C: 857.2
 Target phase: BCC_A2
 Parent phase: FCC_A1
 max. T-step: 20
 dfm-offset: 0

Impose transformations ...

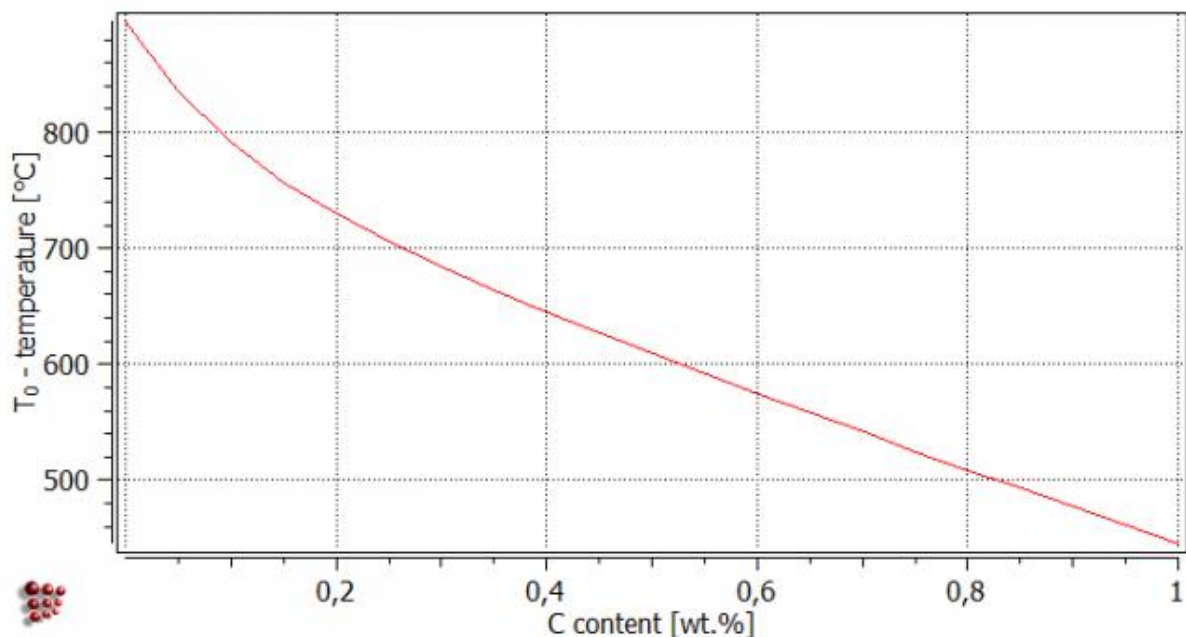
Add ... Remove Edit ...

Cancel Go

There is no need to create a new plot in order to display the graph for the T_0 -temperature dependence for varying carbon content. The T_0 - temperature line in the figure can be simply changed by **switching** from '**T0-chromium**' buffer to the '**T0-carbon**' buffer **in the options window**.

option	value
core buffer	T0-chromium
default x-data	T0-chromium
▶ default x-axis	T0-carbon
plot columns	auto
style sheet	col_no_symb
▶ Font	
▶ Line thickness	
▲ plots	
▲ plot #0	id=01
title	
▶ legend	
▶ axes	
▶ grid	
▶ series	

Afterwards, the x- and y-axes must be rescaled and in the case of the x-axis renamed. So the result looks as follows.

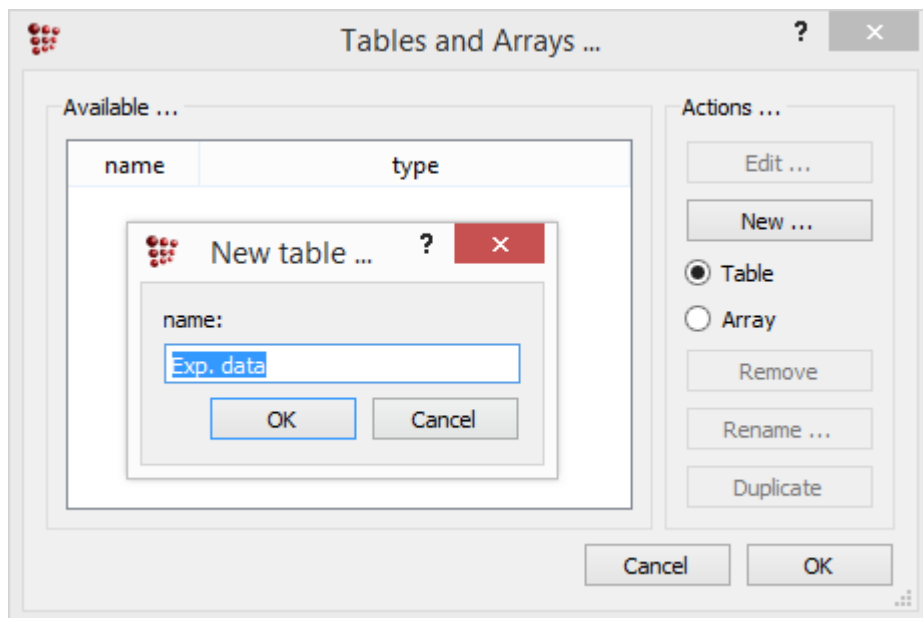


The strong dependence of the T_0 - temperature on the carbon content is evident. This is reflected in the strong influence of carbon on the martensite start temperature.

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 '**T0 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**'.

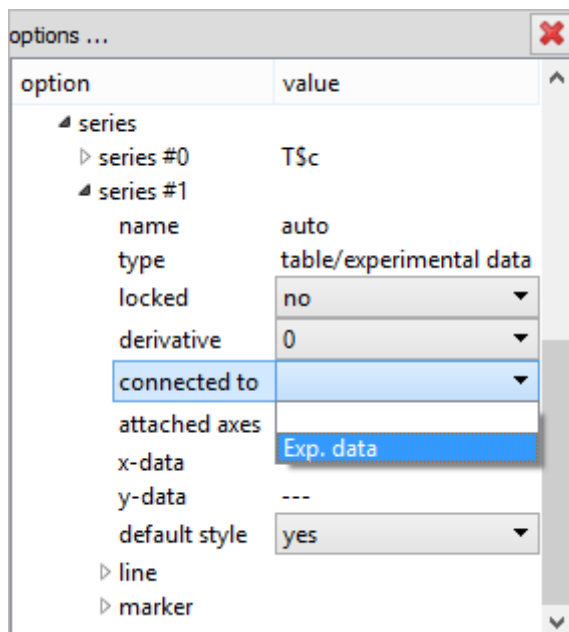


After selecting '**Edit ...**', enter the following measured martensite start temperatures into the table or copy them from a file ([the file is here](#), or here (.txt)).

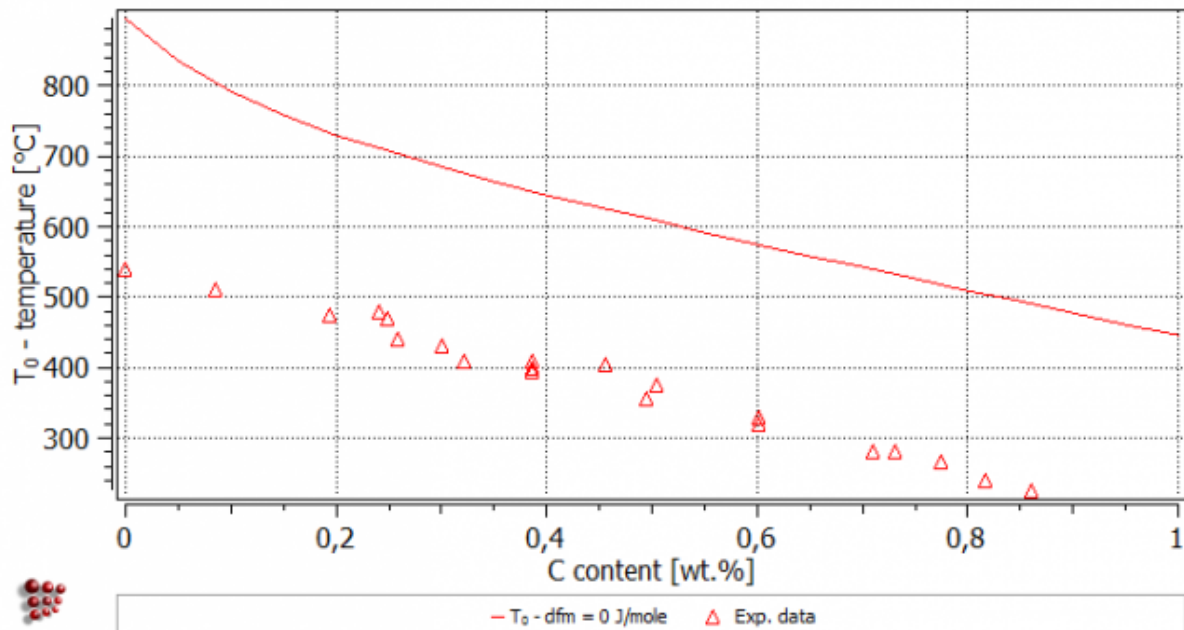
Carbon content [wt%]	Martensite start temperature [°C]
0	540
0.086	510
0.1936	475
0.2409	480
0.2495	470
0.2581	440
0.3011	430
0.3226	410
0.3871	410
0.3871	400

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](#)).



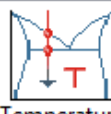
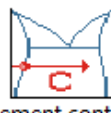
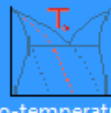
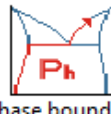

Edit the legend and the series names. The result looks as follows.



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 stepped 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:

Step equilibrium ...

Type ...

 Temperature
 Element content
 **To-temperature**
 Phase boundary
 Defect density

Range ...

Start: 1e-009
 Stop: 1
 Step interval: ☒ linear ☐ logarithmic
 -0,05

☐ vary T only, do not evaluate equilibrium

vary ...
☒ global comp. ☐ paraeq. u-constr.

Boundary conditions ...
 element: C
 temperature C: 857.2
 Target phase: BCC_A2
 Parent phase: FCC_A1
 max. T-step: 20
 dfm-offset: 1200

Options ...

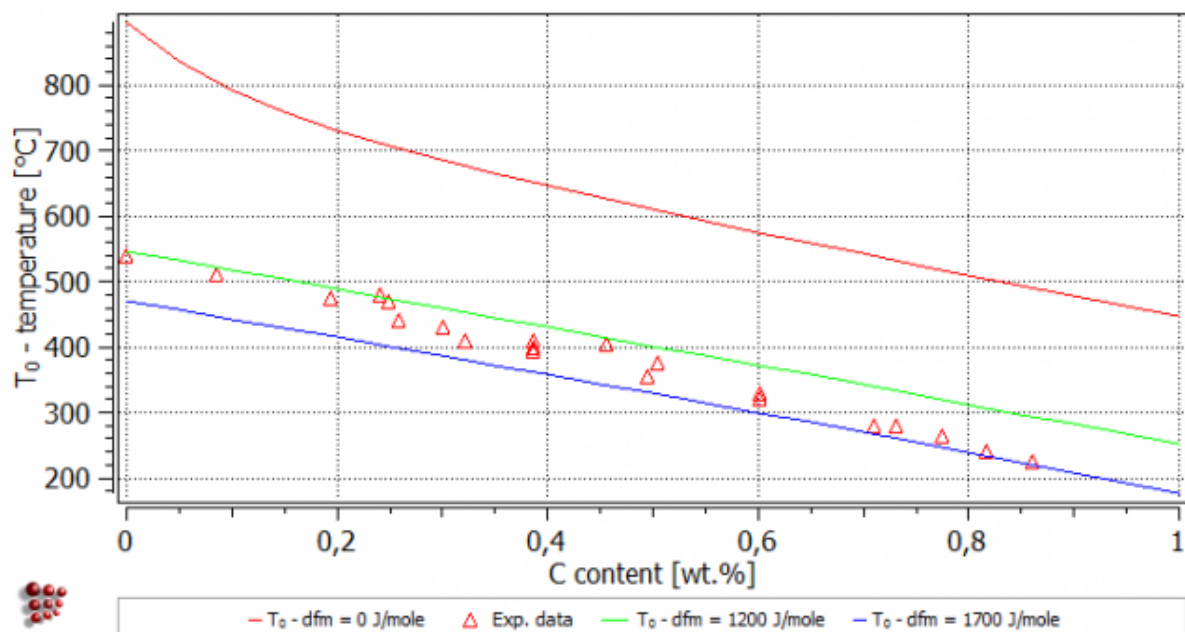
☒ Temperatures in Celsius
☒ Composition in weight percent
☐ Append
☐ Append w/o load
☐ Reverse sort order
☐ Automatically save
☒ Force identical composition

Impose transformations ...

Add ... Remove Edit ...

Cancel Go

Drag and drop the '**T₀c**' 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. Change the plot buffer to '**T₀ with offset**' in the '**options**' window. 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.

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 6.00 rel 0.100
license: free
database: mc_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 $C_{S,i}$).

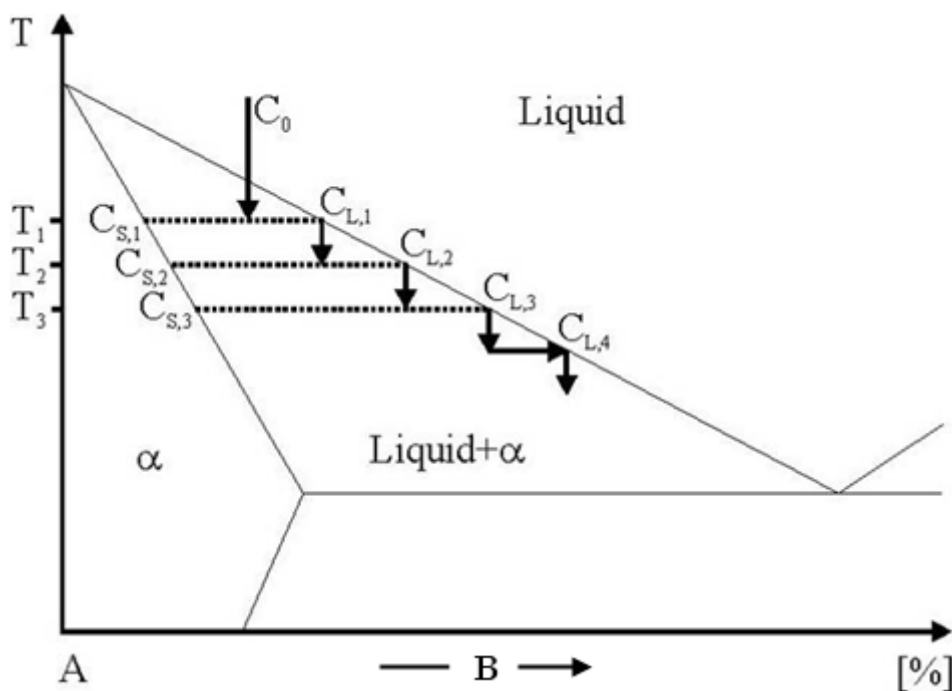


Fig.1: Scheme of Scheil solidification of a hypothetic Fe-C alloy. During solidification the actual liquid phase, beginning with C_0 , is undercooled and solidifies according to the lever rule enriching the liquid phase with solute atoms

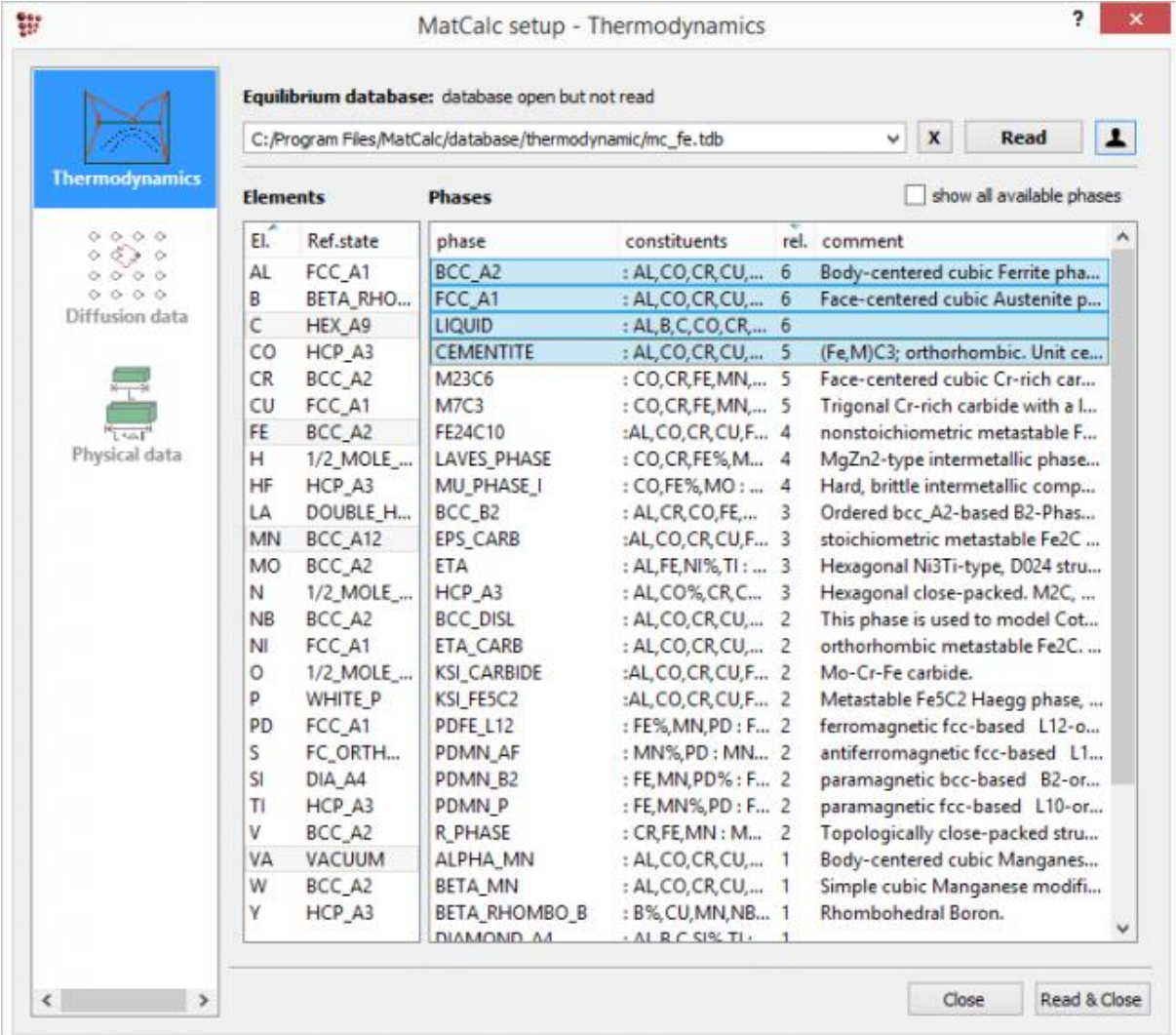
When solidification is finished, the microstructure of the solid phase shows a composition gradient from the regions where the solidification started (centre of the dendrite) to the areas

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_fe.tdb**) define the elements **Fe**, **Mn** and **C** and the phases **liquid**, **BCC_A2** (ferrite), **FCC_A1** (austenite) and **Cementite**.



MatCalc setup - Thermodynamics

Equilibrium database: database open but not read

C:/Program Files/MatCalc/database/thermodynamic/mc_fe.tdb

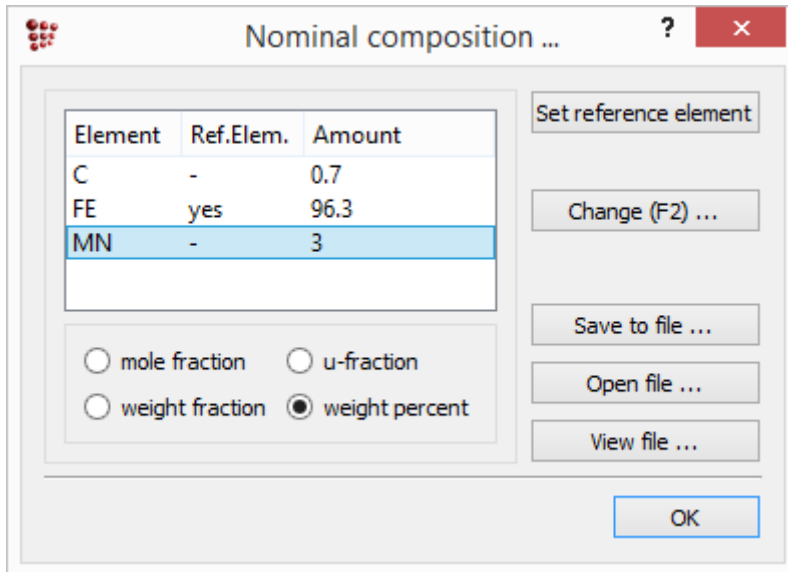
Read

show all available phases

El.	Ref.state	phase	constituents	rel.	comment
AL	FCC_A1	BCC_A2	: AL, CO, CR, CU, ...	6	Body-centered cubic Ferrite pha...
B	BETA_RHO...	FCC_A1	: AL, CO, CR, CU, ...	6	Face-centered cubic Austenite p...
C	HEX_A9	LIQUID	: AL, B, C, CO, CR, ...	6	
CO	HCP_A3	CEMENTITE	: AL, CO, CR, CU, ...	5	(Fe,M)C ₃ ; orthorhombic. Unit ce...
CR	BCC_A2	M23C6	: CO, CR, FE, MN, ...	5	Face-centered cubic Cr-rich car...
CU	FCC_A1	M7C3	: CO, CR, FE, MN, ...	5	Trigonal Cr-rich carbide with a l...
FE	BCC_A2	FE24C10	: AL, CO, CR, CU, F...	4	nonstoichiometric metastable F...
H	1/2_MOLE...	LAVES_PHASE	: CO, CR, FE%, M...	4	MgZn ₂ -type intermetallic phase...
HF	HCP_A3	MU_PHASE_I	: CO, FE%, MO : ...	4	Hard, brittle intermetallic comp...
LA	DOUBLE_H...	BCC_B2	: AL, CR, CO, FE, ...	3	Ordered bcc_A2-based B2-Phas...
MN	BCC_A12	EPS_CARB	: AL, CO, CR, CU, F...	3	stoichiometric metastable Fe ₂ C ...
MO	BCC_A2	ETA	: AL, FE, NI%, TI : ...	3	Hexagonal Ni ₃ Ti-type, D0 ₂₄ stru...
N	1/2_MOLE...	HCP_A3	: AL, CO%, CR, C...	3	Hexagonal close-packed. M2C, ...
NB	BCC_A2	BCC_DISL	: AL, CO, CR, CU, ...	2	This phase is used to model Cot...
NI	FCC_A1	ETA_CARB	: AL, CO, CR, CU, ...	2	orthorhombic metastable Fe ₂ C. ...
O	1/2_MOLE...	KSI_CARBIIDE	: AL, CO, CR, CU, F...	2	Mo-Cr-Fe carbide.
P	WHITE_P	KSI_FE5C2	: AL, CO, CR, CU, F...	2	Metastable Fe ₅ C ₂ Haegg phase, ...
PD	FCC_A1	PDFE_L12	: FE%, MN, PD : F...	2	ferromagnetic fcc-based L12-o...
S	FC_ORTH...	PDMN_AF	: MN%, PD : MN...	2	antiferromagnetic fcc-based L1...
SI	DIA_A4	PDMN_B2	: FE, MN, PD% : F...	2	paramagnetic bcc-based B2-or...
TI	HCP_A3	PDMN_P	: FE, MN%, PD : F...	2	paramagnetic fcc-based L10-or...
V	BCC_A2	R_PHASE	: CR, FE, MN : M...	2	Topologically close-packed stru...
VA	VACUUM	ALPHA_MN	: AL, CO, CR, CU, ...	1	Body-centered cubic Manganes...
W	BCC_A2	BETA_MN	: AL, CO, CR, CU, ...	1	Simple cubic Manganese modifi...
Y	HCP_A3	BETA_RHOMBO_B	: B%, CU, MN, NB...	1	Rhombohedral Boron.
		DIAMOND_A4	: AL, B, C, SI%, TI...	1	

Close Read & Close

Enter the system composition in weight percent as listed in the subsequent figure selecting '**Global Composition ...**' or pressing the **F7** key.



The dialog box titled "Nominal composition ..." contains a table with the following data:

Element	Ref.Element	Amount
C	-	0.7
FE	yes	96.3
MN	-	3

Below the table are four radio buttons for units:
☐ mole fraction ☐ u-fraction
☐ weight fraction ☒ weight percent

On the right side of the dialog are buttons: "Set reference element", "Change (F2) ...", "Save to file ...", "Open file ...", "View file ...", and "OK".

Set initial values with '**Calc**'→'**Set start values**' or **Ctrl+Shift+F**. Calculate equilibrium at 1600°C. The results in the '**Phase summary**' window are

```

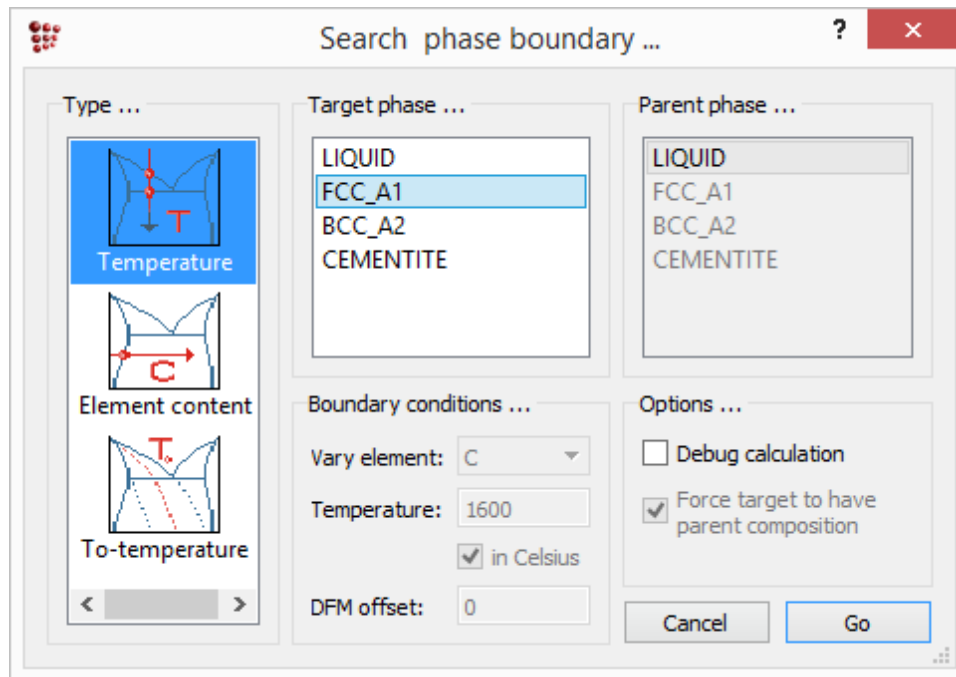
LIQUID *      act      1,00000e+000 dfm: +0,00000e+000

### inactive ###

BCC_A2        - OK -    0,00000e+000 dfm: -1,02376e+003
FCC_A1        - OK -    0,00000e+000 dfm: -1,08279e+003
CEMENTITE     - OK -    0,00000e+000 dfm: -1,28109e+004
  
```

STEP 2: CARRY OUT A SCHEIL CALCULATION

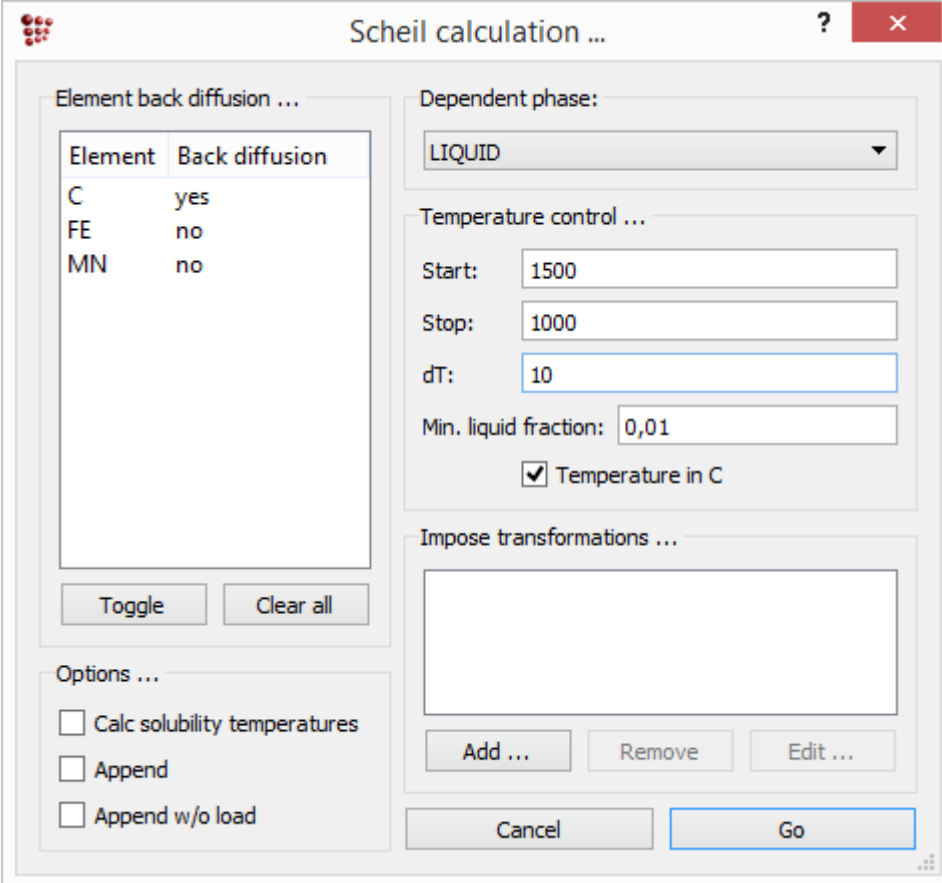
Since we expect austenite to be the first phase to form on solidification, let us first look for the solubility temperature of this phase. Select '**Calc - Search phase boundary ...**' or press **Ctrl+Shift+T** and select **FCC_A1** as target phase.



Press '**Go**':

```
Tsol 'FCC_A1': 1471,08 C (1744,24 K) iter: 4, time used: 0,03 s
```

The first solid phase becomes stable at **1471.08°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**.



Scheil calculation ...

Element back diffusion ...

Element	Back diffusion
C	yes
FE	no
MN	no

Dependent phase:
LIQUID

Temperature control ...

Start: 1500
Stop: 1000
dT: 10
Min. liquid fraction: 0,01
☒ Temperature in C

Options ...

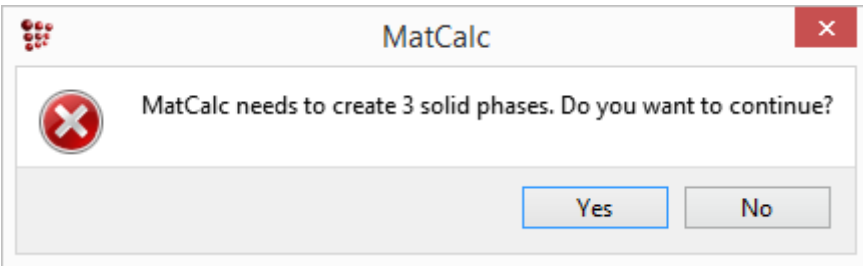
☐ Calc solubility temperatures
☐ Append
☐ Append w/o load

Impose transformations ...

Add ... Remove Edit ...

Cancel Go

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



MatCalc

MatCalc needs to create 3 solid phases. Do you want to continue?

Yes No

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 ... - OK -
Searching initial equilibrium ...
1, 0,05 s, 1500,00 C (1773,16 K), its 2, f=1,00000000, LIQUID
...
```

```

3, 0,05 s, 1480,00 C (1753,16 K), its 2, f=1,00000000, LIQUID
4, 0,05 s, 1470,00 C (1743,16 K), its 5, f=0,97044923, LIQUID FCC_A1
...
12, 0,08 s, 1390,00 C (1663,16 K), its 6, f=0,25234865, LIQUID FCC_A1
13, 0,08 s, 1380,00 C (1653,16 K), its 6, f=0,22795930, LIQUID FCC_A1
14, 0,08 s, 1370,00 C (1643,16 K), its 6, f=0,20745452, LIQUID FCC_A1
15, 0,08 s, 1360,00 C (1633,16 K), its 6, f=0,19000907, LIQUID FCC_A1
...
39, 0,17 s, 1120,00 C (1393,16 K), its 5, f=0,05686078, LIQUID FCC_A1
40, 0,17 s, 1110,00 C (1383,16 K), its 11, f=0,00000000, FCC_A1 CEMENTITE
fraction of phase 'LIQUID' smaller than 0,01. Calc finished

Steps:41, CalcTime: 0,17 s

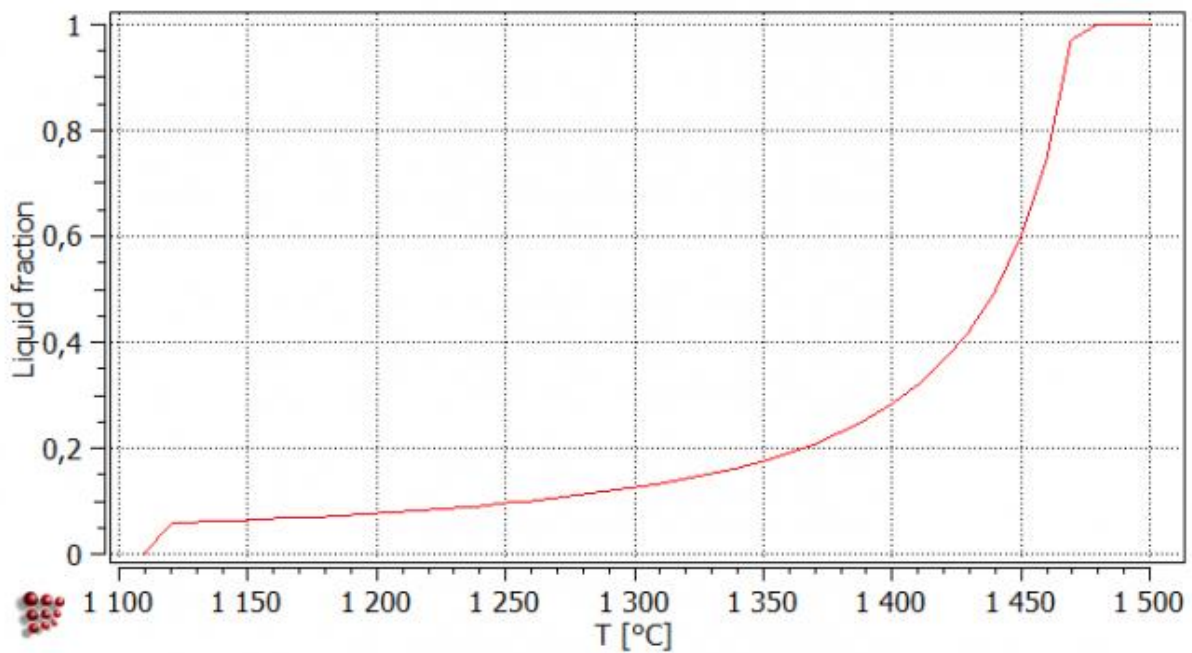
AktStepVal: 1383,160000

- OK -

```

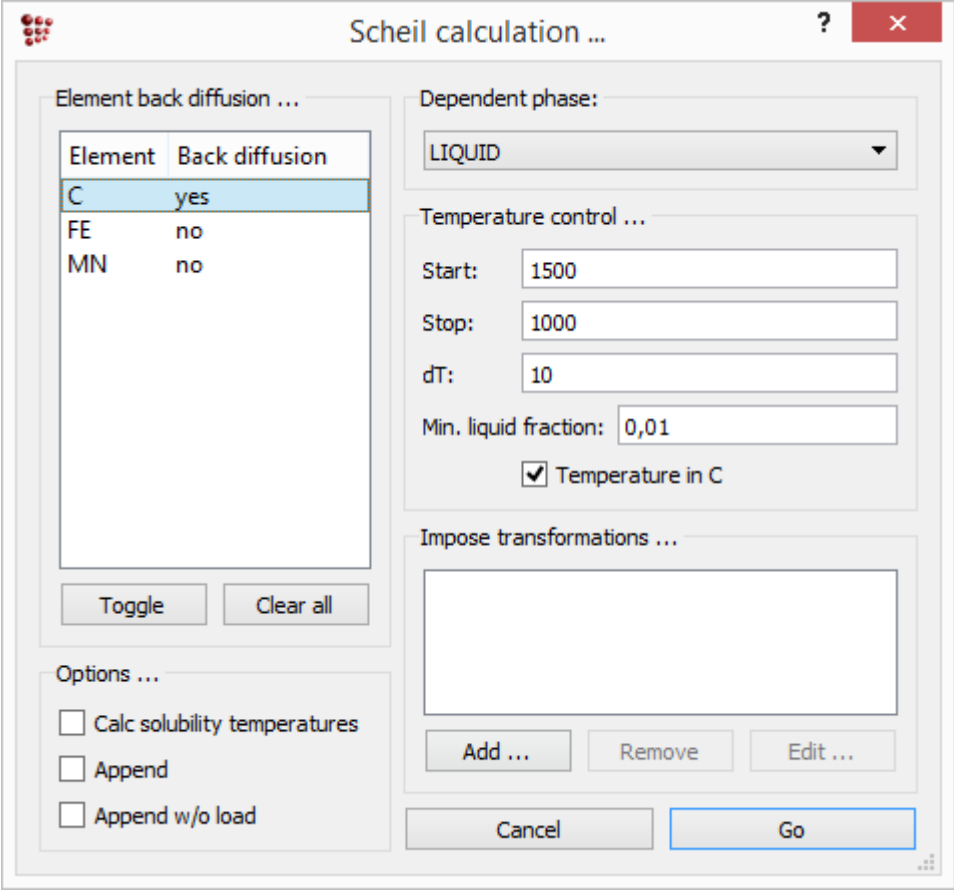
The current value of the fraction liquid at each temperature step is displayed with '**f=xxx**' in each line. The final eutectic is reached at $T=1110^{\circ}\text{C}$. When the fraction liquid comes **below 0,01 (minimum liquid fraction)**, the dependent phase is dissolved and the calculation is finished. 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 $^{\circ}\text{C}$ 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 lose 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'**.



Element back diffusion ...

Element	Back diffusion
C	yes
FE	no
MN	no

Dependent phase: LIQUID

Temperature control ...

Start: 1500

Stop: 1000

dT: 10

Min. liquid fraction: 0,01

☒ Temperature in C

Options ...

☐ Calc solubility temperatures

☐ Append

☐ Append w/o load

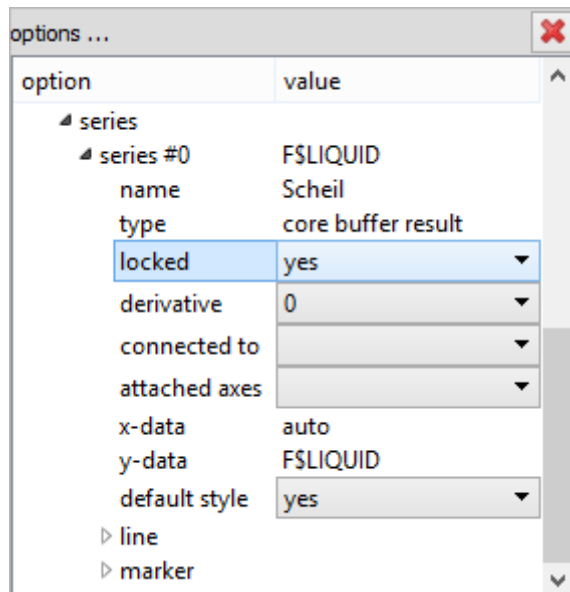
Impose transformations ...

Add ... Remove Edit ...

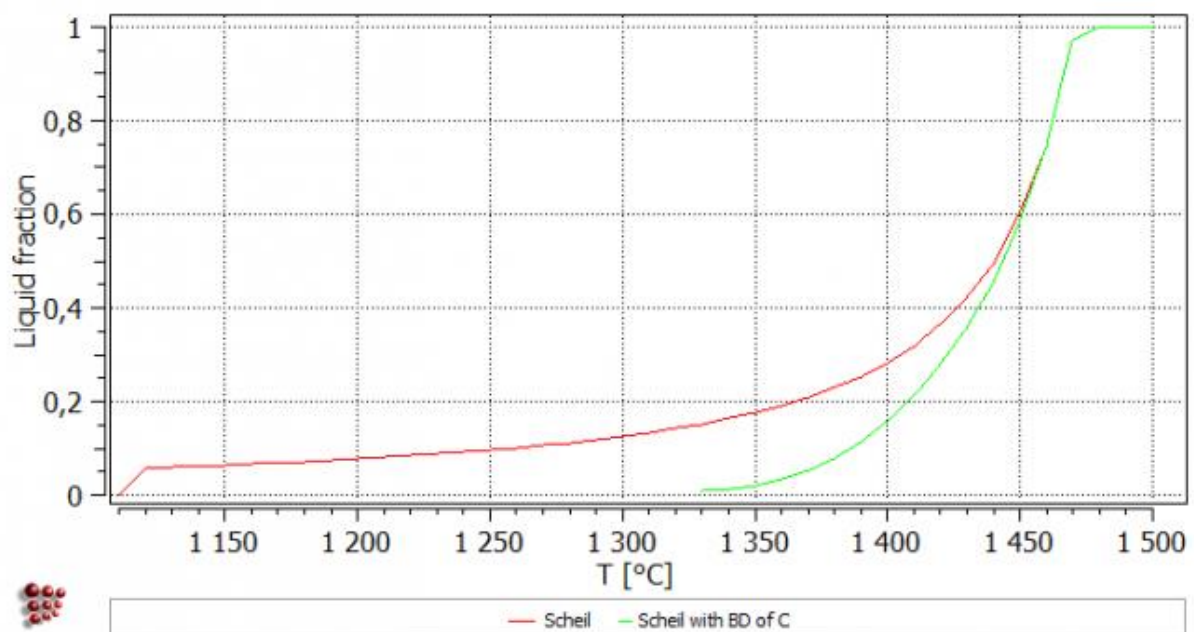
Cancel Go

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**'.

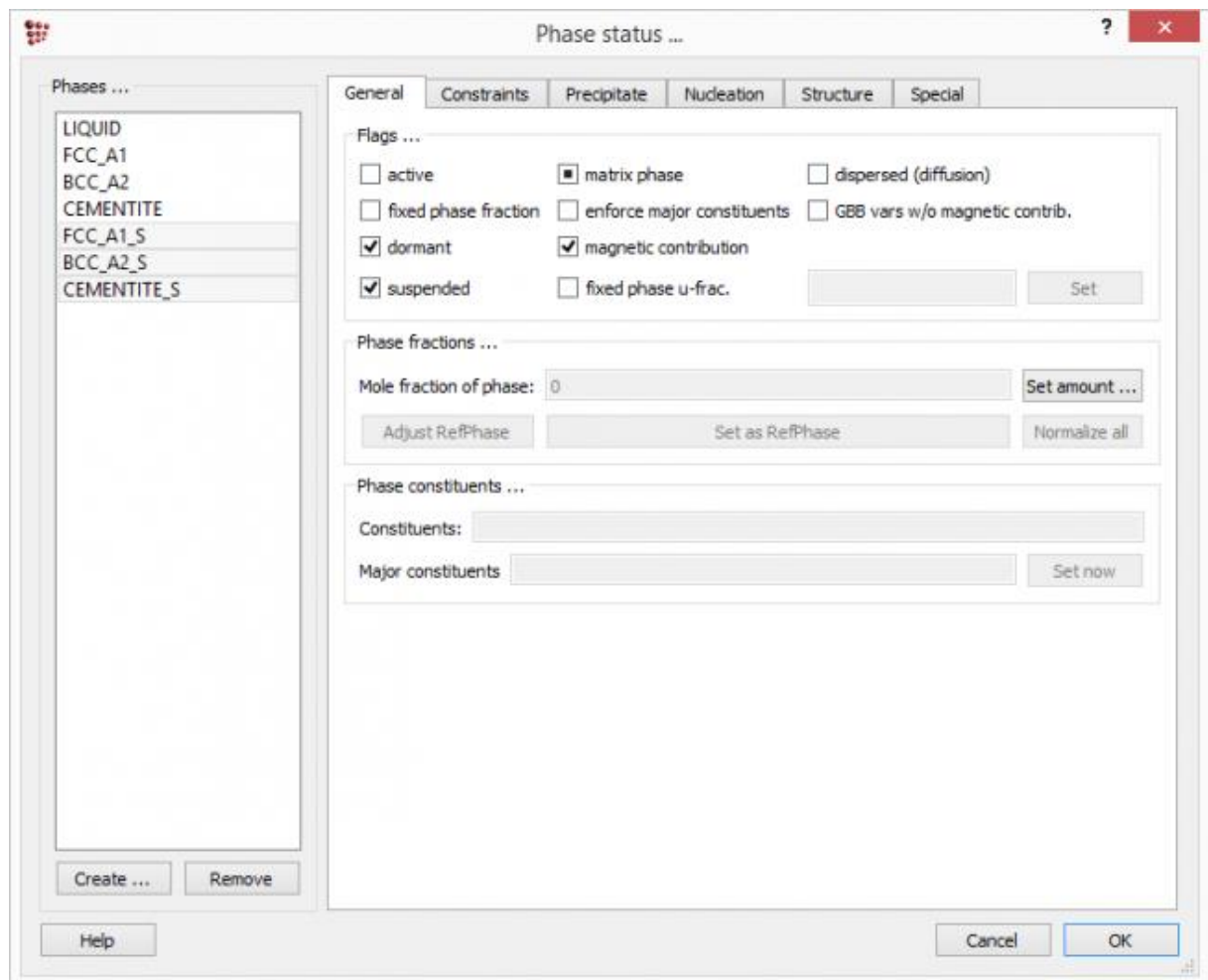


Then, we make sure that the just created buffer ('**Scheil with BD of C**') is selected as current buffer for the plot in the options window and drag and drop the '**F\$LIQUID**' variable into the plot (note that alternatively you can use the 'Lock and duplicate series' option accessible via the right 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.

Step equilibrium ...

Type ...

Temperature

Element content

To-temperature

Phase boundary

Defect density

Range ...

Start: 1500

Stop: 1350

Step interval: ☒ linear ☐ logarithmic

☐ vary T only, do not evaluate equilibrium

vary ...

☒ global comp. ☐ paraeq. u-constr.

Boundary conditions ...

element: C

temperature C: 1471.08

Target phase: LIQUID

Parent phase: LIQUID

max. T-step: 20

dfm-offset: 0

Options ...

☒ Temperatures in Celsius

☒ Composition in weight percent

☐ Append

☐ Append w/o load

☐ Reverse sort order

☐ Automatically save

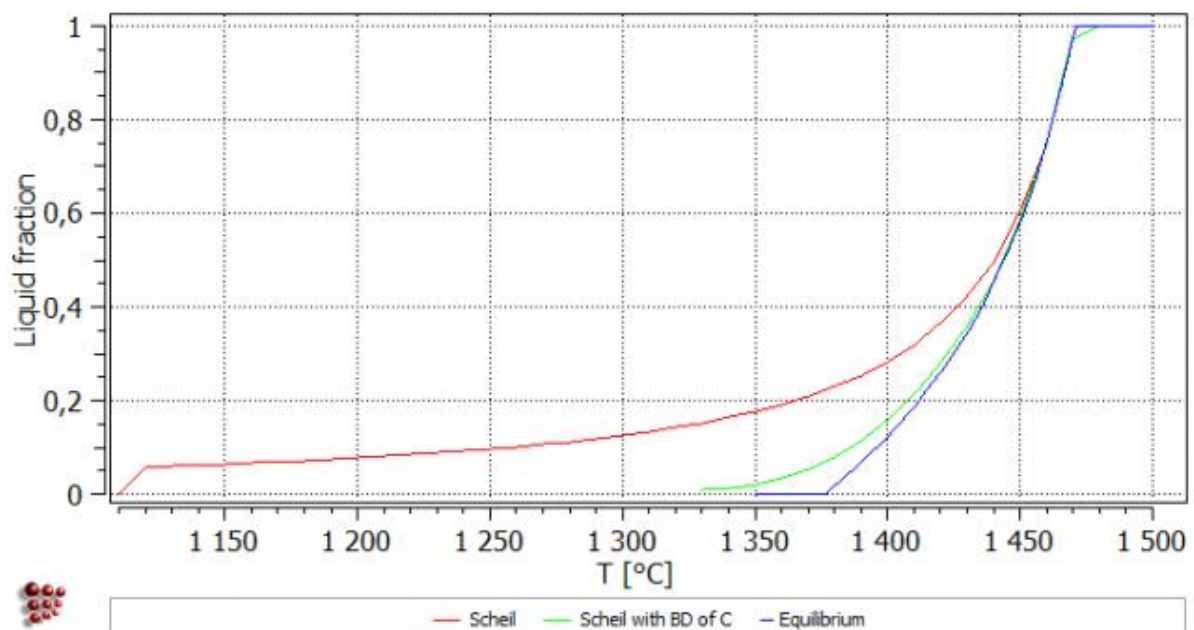
☐ Force identical composition

Impose transformations ...

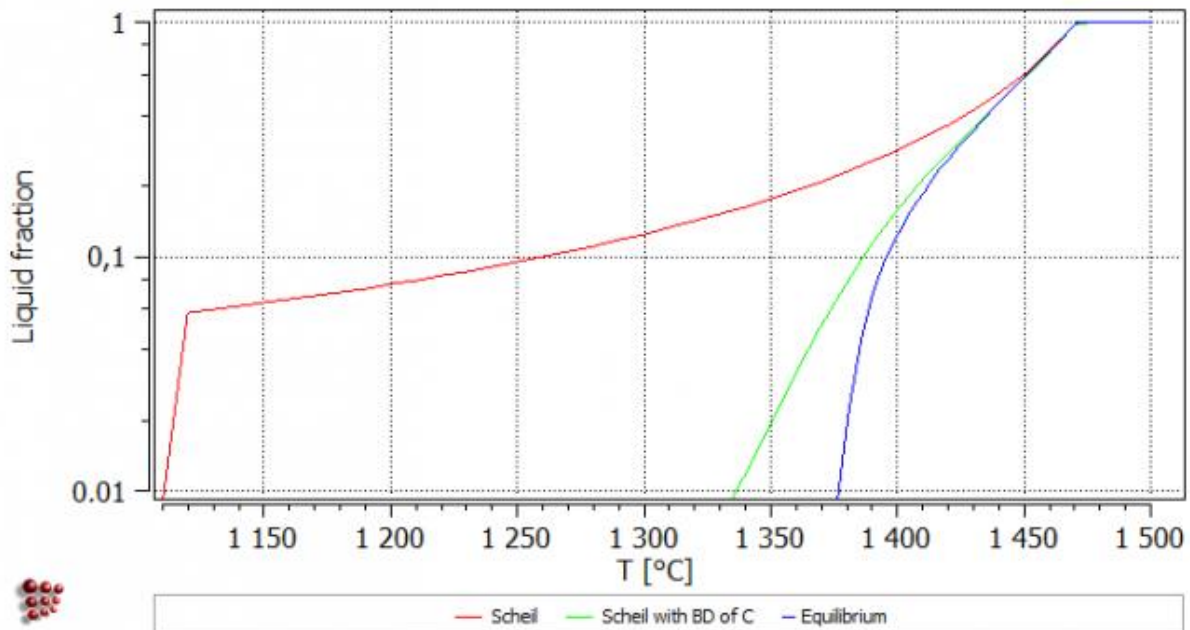
Add ... Remove Edit ...

Cancel Go

Lock the last series ('Scheil with BD of C'). Change the buffer to be used in the diagram window to **'Equilibrium'** and drag and drop the **'F\$LIQUID'** variable into the plot. 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.

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 6.00 rel 0.100

license: free

database: mc_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

GENERAL REMARK TO 6.00.0100 VERSION

Due to some development activities, the commands are to be typed into the 'MatCalc 5 console' window - this are the lines beginning here with 'MCORE:'. The output messages are displayed in the 'console' window, as always.

BASICS

GETTING HELP AND LISTING AVAILABLE COMMANDS

Typing '?' or 'HELP_WORKSPACE' in the 'MatCalc 5 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           SET_LICENSE_FILEPATH
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
CALC_PARTITION_RATIO       <<CORE>>                    <<NODES>>
<<SYMBOLIC>>               <<IO>>                      <<PRECIPITATION>>
<<STATE>>                  <<BUFFER>>                  <<TABLES/ARRAYS>>
<<TRANSFORMATIONS>>       <<HEAT_TREATMENTS>>        <<EXPORT>>

```

The '**mc_core**' 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/core)> $ phase details: create and move

<script(0/core)> new-gui-window a6

<script(0/core)> move-gui-window . 500 0 500 450move-gui-window window-id=. x-
axis=500 y-axis=0 width=500 height=450

<script(0/core)> $ phase summary: create and move

<script(0/core)> new-gui-window a5

<script(0/core)> move-gui-window . 0 0 450 300move-gui-window window-id=. x-axis=0
y-axis=0 width=450 height=300

<script(0/core)> $ clear modified-flag

<script(0/core)> set-workspace-property m n

<script(0/core)> $ ready ...
```

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). Type '**mc_fe.tdb**' to select the improved database.

```
MCORE: open_thermodyn_database

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

```
opening database 'mc_fe.tdb' ...
```

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/:
```

Type in '**e**', to show the content of the opened equilibrium database

```
MCORE: list_database_contents
```

```
(e)quilib/(d)iffusion/(p)hysical /e/:
```

```
equilibrium database file: mc_fe.tdb
```

```
# of elements in database: 25
```

```
      VA, AL, B, C, CO, CR, CU, FE, H, HF, LA, MN, MO, N, NB, NI, O, P, PD, S, SI,  
      TI, V, W, Y
```

```
# of phases in database: 122
```

LIQUID	FCC_A1	BCC_A2
H_BCC	BCC_DISL	HCP_A3
ALPHA_MN	BETA_MN	BETA_RHOMBO_B
DIAMOND_A4	GRAPHITE	BCC_B2
CHI_A12	CO3MO	CO3V
COV3	CR3MN5	G_PHASE
LAVES_PHASE	MNNI	MNNI2
MNNI_T3	MU_PHASE	MU_PHASE_I
ETA	NITI2	PI_PHASE
R_PHASE	SIGMA	FE17Y2
NI5Y	PDFE_L12	PDMN_AF
PDMN_P	PDMN_B2	PD2MN
PD3MN	PD5MN3	PD6FE5MN2
CEMENTITE	CR2VC2	K_CARB

KSI_CARBIDE	M3C2	M6C
M7C3	M12C	M23C6
MOC_ETA	V3C2	WC
EPS_CARB	ETA_CARB	FE24C10
KSI_FE5C2	ALN	ALN_EQU
BN_HP4	CR3NI2SIN	FE4N
MN6N4	MN6N5	MNSIN2
SI3N4	ZET	CRB
CR2B	CR5B3	FEB
FENBB	FE3NB3B4	M2B
MNB2	MNB4	O_MN2B
MN3B4	MOB	MOB2
MO2M1B2	NBB	NB3B2
M5B6	TIB	TIB2
TI3B4	A_CHALC	ANILITE
B_CHALC	COVELLITE	CU2S
DIGENITE	DISULF	DJURLEITE
FC_MONO	FC_ORTHO	FES_P
MNS_Q	PYRR	TIS
TI4C2S2	CORUND	HALITE
HF102_M	HF102_T	HF102_C
LA2O3_A	LA2O3_H	LA2O3_C
SIO2	SPINEL	TIO2
TI2O3	TRID	Y2O3_C
Y2O3_H	YALO3	Y4AL2O9
Y2TIO5	Y2TI2O7	O1_GAS
M2P	M3P	

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_a2 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
```

```
reading thermodynamic data 'mc_fe.tdb' ...
```

```
collecting symbols 'mc_fe.tdb' ...
```

```
elements: VA C FEhases: LIQUID FCC_A1 BCC_A2 CEMENTITE
```

```
Gibbs: 4 Phases / 0 Composition-Set(s) created
```

```
Gibbs: 30 functions linked ...
```

```
Gibbs: T = 1273.160000 K, P = 101325.000000 Pa, moles = 1
```

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
```

```
iter: 13, time used: 0,02 s
```

```
T: 700 C (973,16 K), GibbsEnergy: -39934,665 J
```

```
- OK -
```

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)
```

$$4/(5*3) =$$
$$0.2666666666667$$

```
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/rename/(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
```

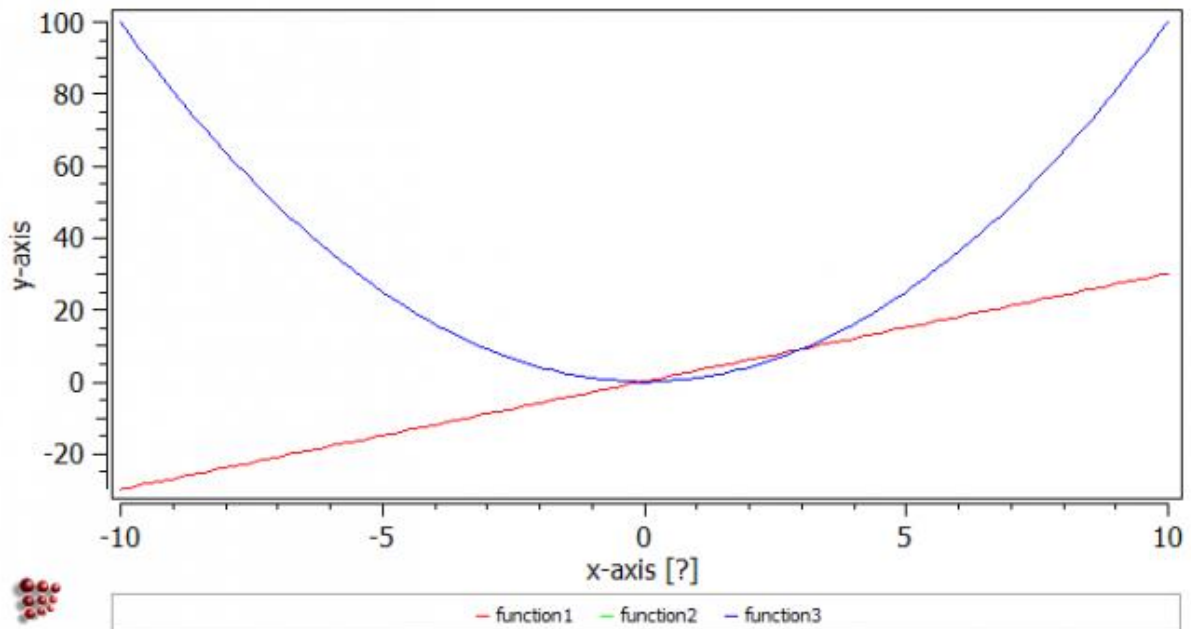
```
definition range /auto/: -10..10
```

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 =
```

```
0,000628639871334
```

```
MCORE: sh function5
```

```
function5 =
```

```
0,0177023706434
```

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, $\text{function4} + \text{function5} = \text{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.

T13: INTRODUCTION TO SCRIPTING - EQUILIBRIUM CALCULATIONS

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

database: mc_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 '**Script** → **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_fe2.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_a2 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 Fe<sub>3</sub>C
```

The major grid lines for x- and y-axis are displayed by these commands:

```
set-plot-option . g m x y $ plot x-axis major grid line
set-plot-option . g m y y $ plot y-axis major grid line
```

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
```

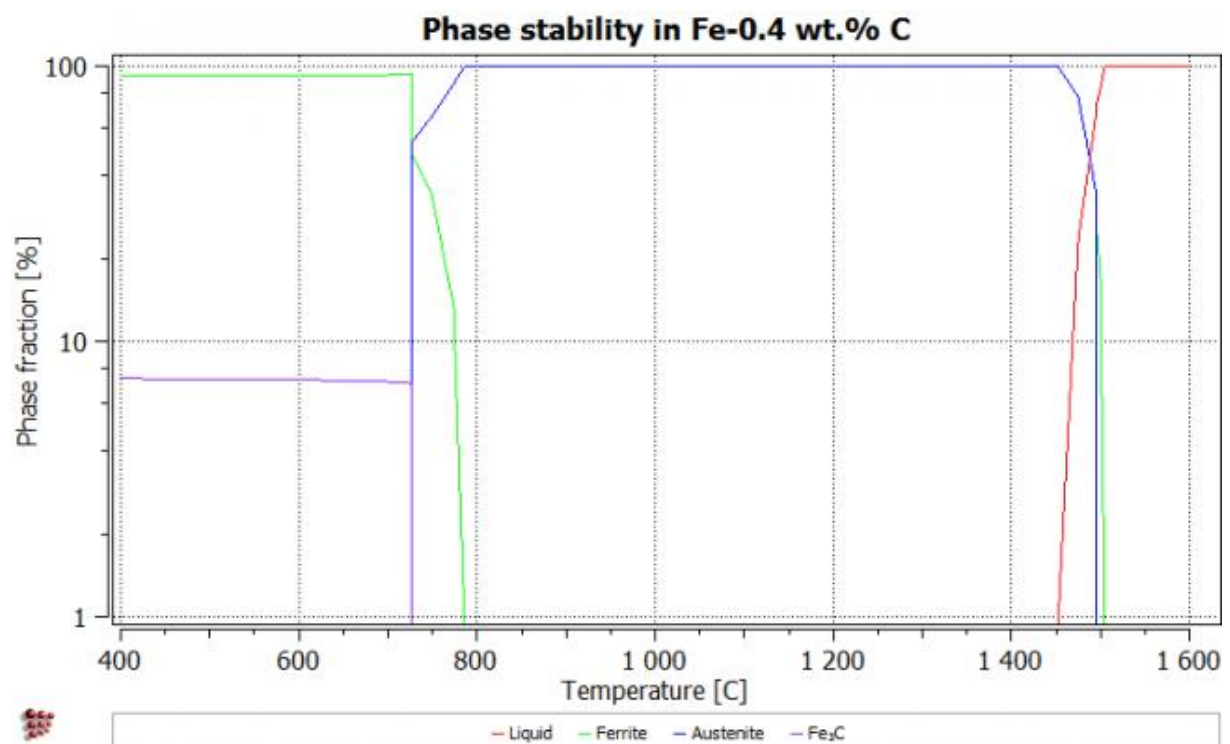


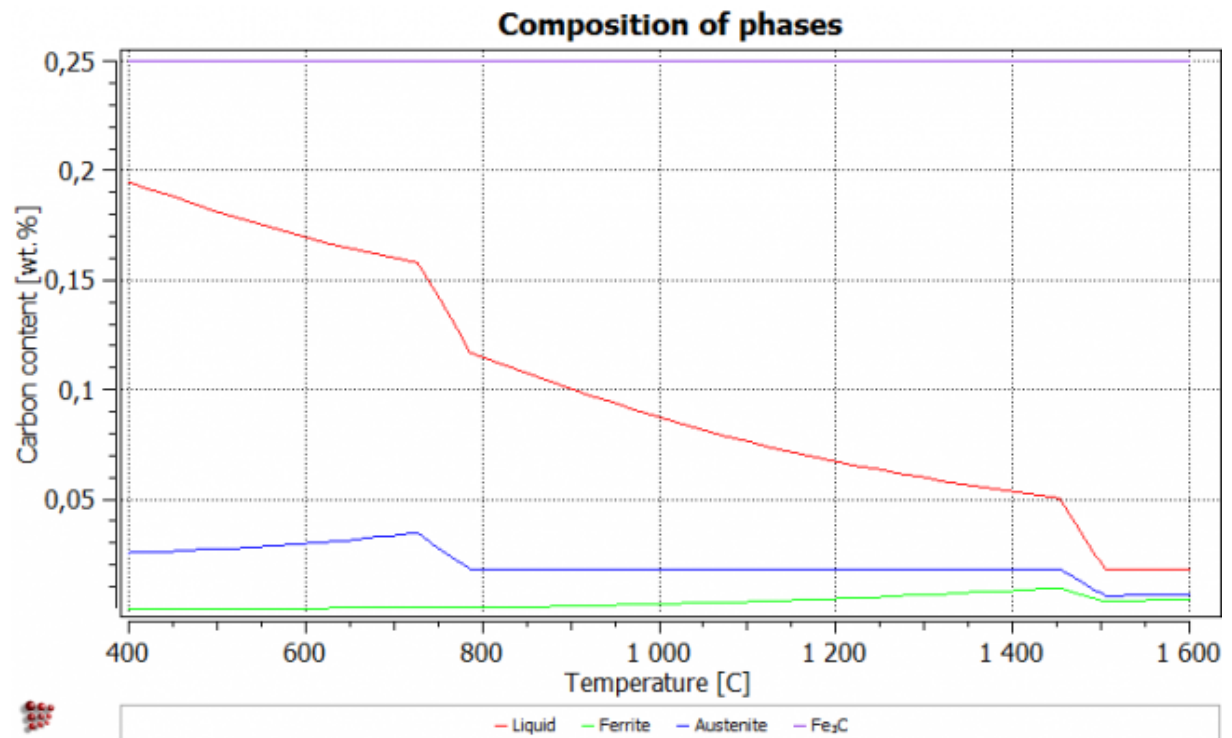
```
set-plot-option . s m -1 x$cementite$C Fe<sub>3</sub>C
set-plot-option . g m x y
set-plot-option . g m y y
```

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:





T14: INTRODUCTION TO PRECIPITATION CALCULATIONS

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

database: mc_fe.tdb; mc_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

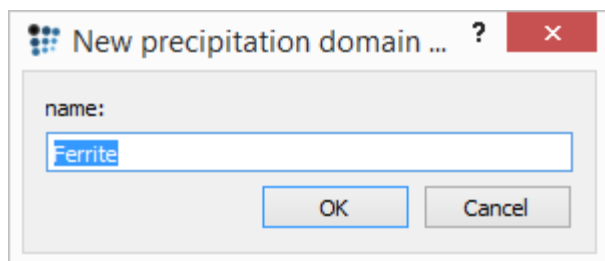
A. THERMODYNAMIC SETUP

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.%.

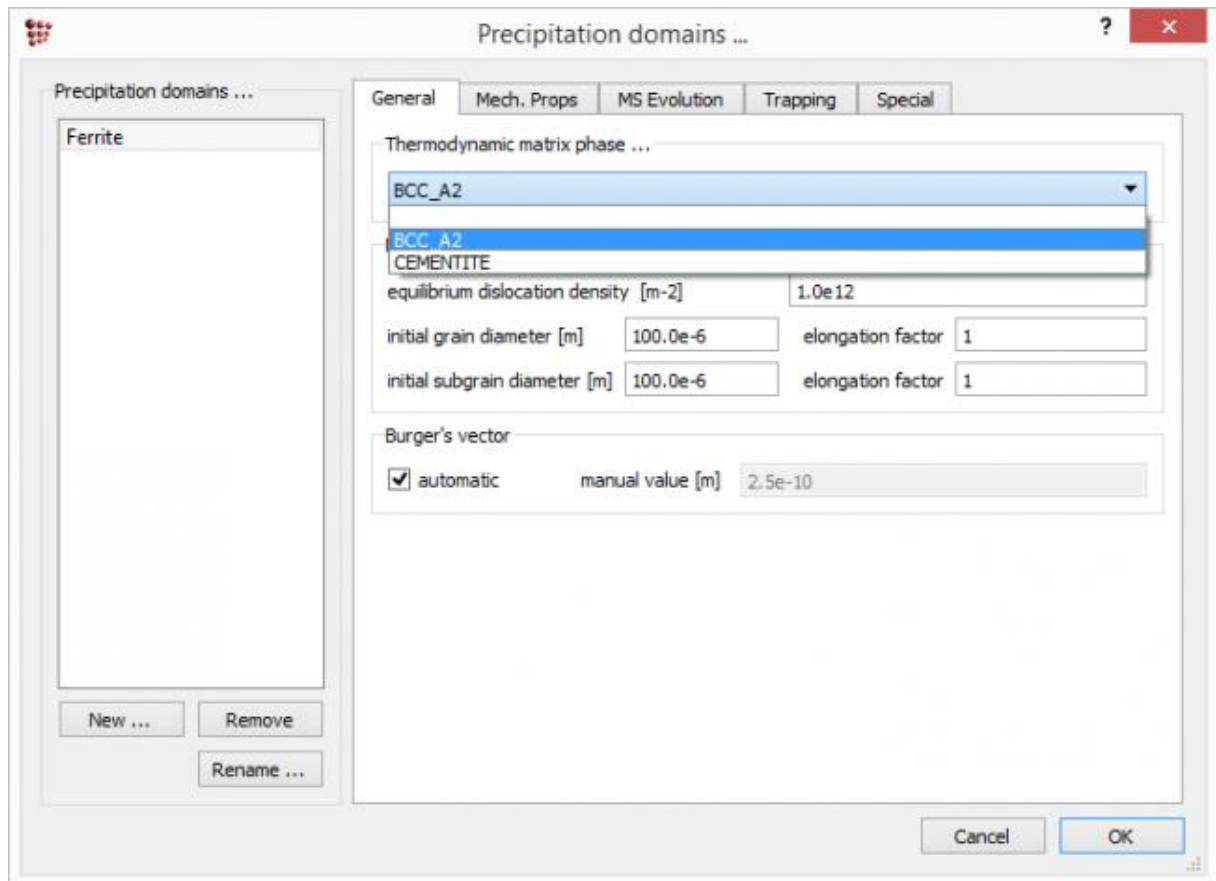
B. PRECIPITATION DOMAIN

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**'.

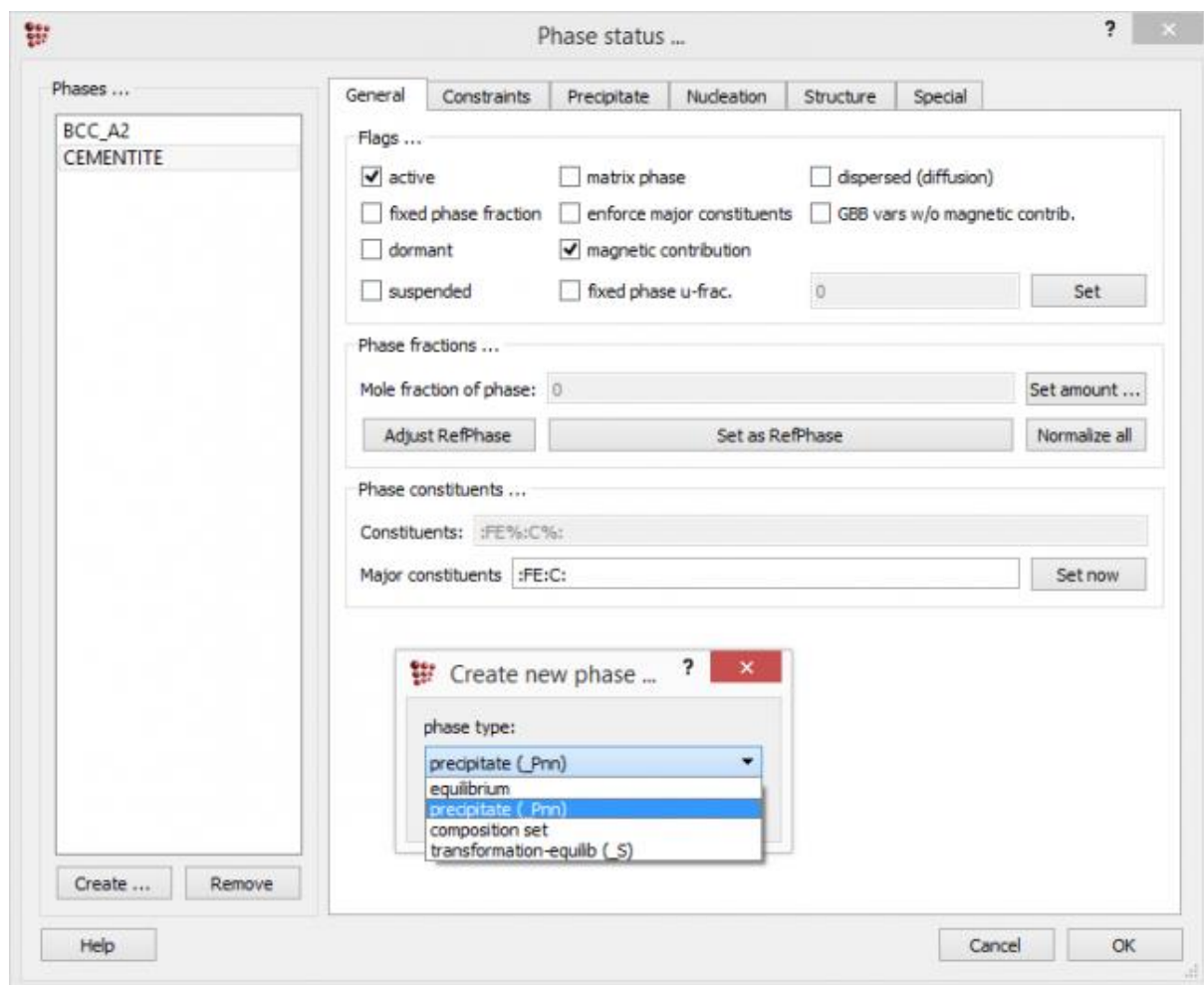


On the '**Phases**' tab, choose '**BCC_A2**' from the drop-box to associate this phase with the newly defined domain. Leave the rest of the settings as they are, and click '**OK**'.

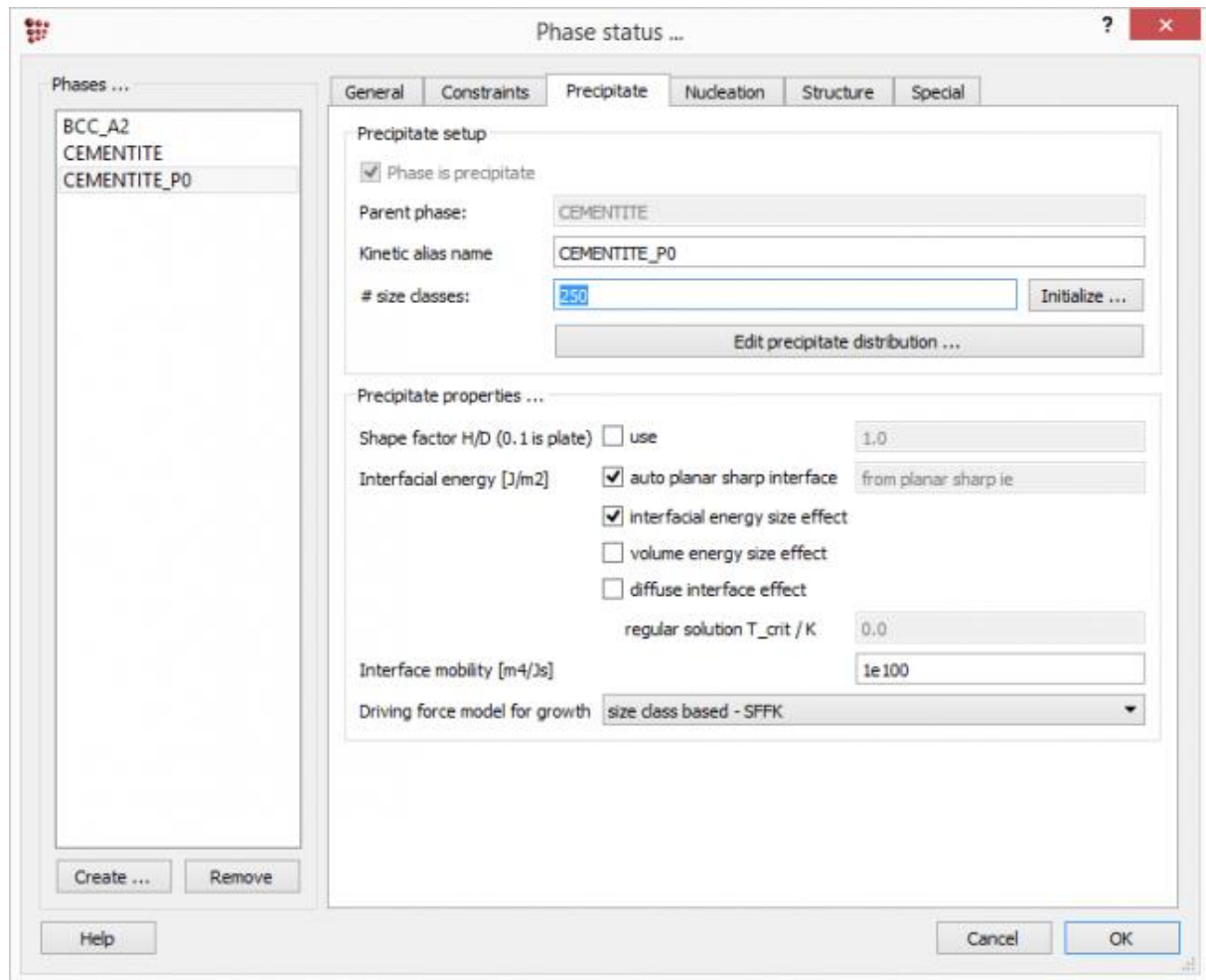


C. PRECIPITATE PHASE

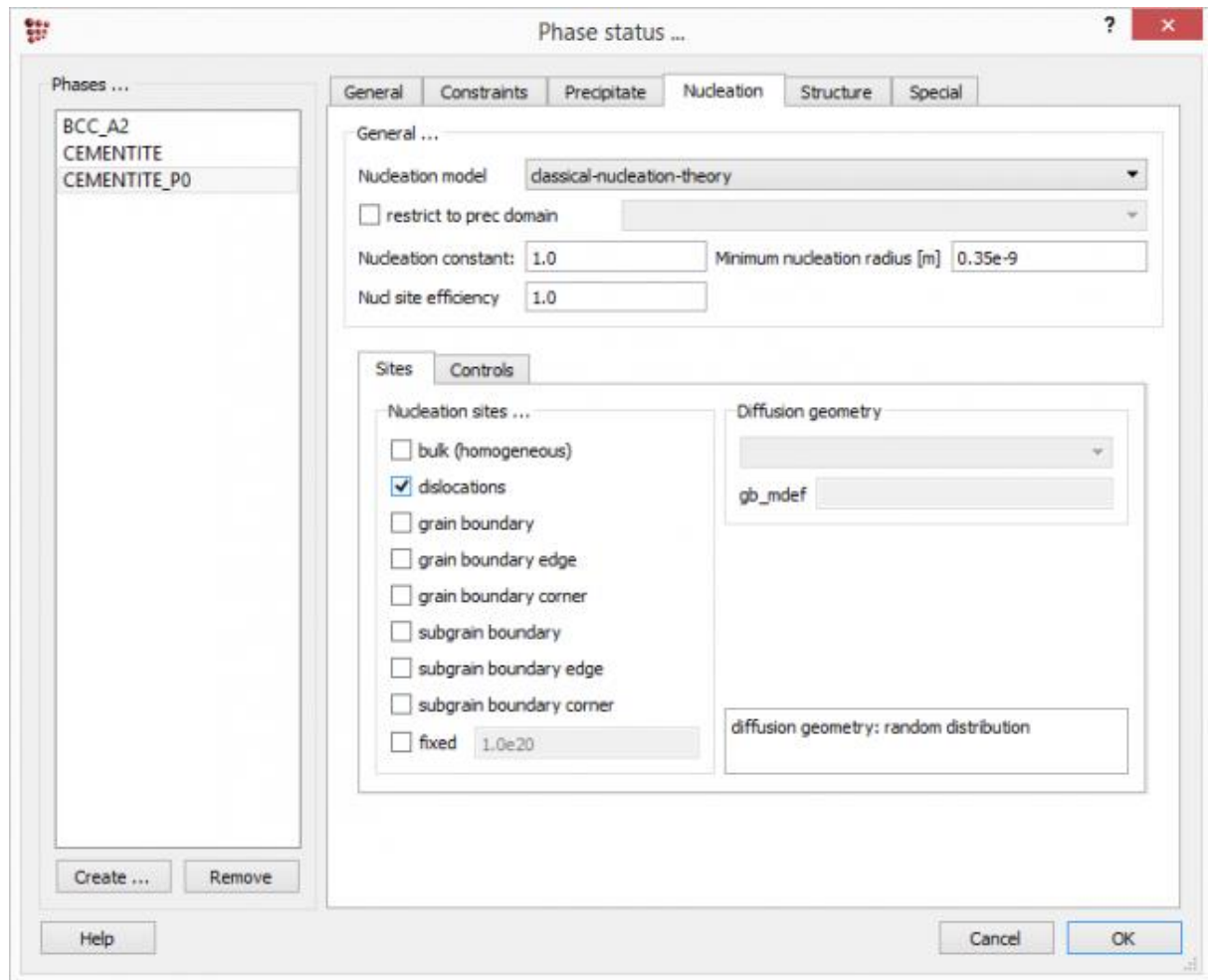
To create the precipitate phase, open '**Global > Phase status**'. In the '**Phases**' list on the left-hand side, select '**CEMENTITE**' and click on '**Create**'. Select '**precipitate (_Pnn)**' from the drop box which opens.



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.

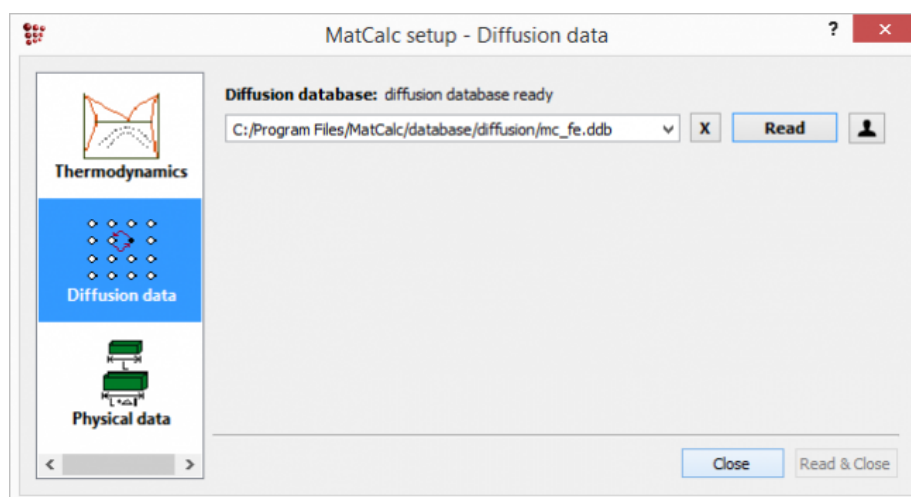


Open the '**Nucleation**' tab and select the '**Sites**' sub-tab. In the '**Nucleation sites...**' part of this tab, remove the tick-mark by '**bulk (homogeneous)**' and instead click in the box beside '**dislocations**'. Click on '**OK**' to save these settings and return to the main screen.



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_fe.ddb**' database. Click on '**Close**'



E. CREATING PLOTS FOR THE OUTPUT

Create a new **'Plot: XY-data'** window. Drag and drop **'F\$CEMENTITE_PO'** from the variables window to this plot. In the **'options'** window, set **'default x-axis'** to **'log'** type. 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_PO'** from the box which opens and click **'OK'**. In the **'options'** window, change the number of **'# size classes'** for this histogram to **'20'**. Switch off the default x-axis (in 'default x-axis', set 'no' for 'use for all plots') and 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'**.


options ...	
option	value
default x-data	StepValue
▾ default x-axis	
use for all plots	no
title	x-axis [?]
type	lin
unit	#NYA
scaling	auto
factor	1
legend position	bottom
# size classes	20
plot columns	auto
style sheet	col_no_symb
▸ Font	
▸ Line thickness	
▾ plots	
▾ plot #0	id=02
title	
# size classes	auto
histogram type	number
scale frequency	no
scale radius	no
▸ legend	
▾ axes	
▾ x-axis	
title	Precipitate radius [nm]
type	lin
unit	#NYA
scaling	auto
scaling in segments	no
factor	1e+009
▾ y-axis	
title	Number of precipitates
type	lin
unit	#NYA
scaling	auto
scaling in segments	no
factor	1
▸ 2nd-x-axis	
▸ 2nd-y-axis	
▸ grid	
▸ series	

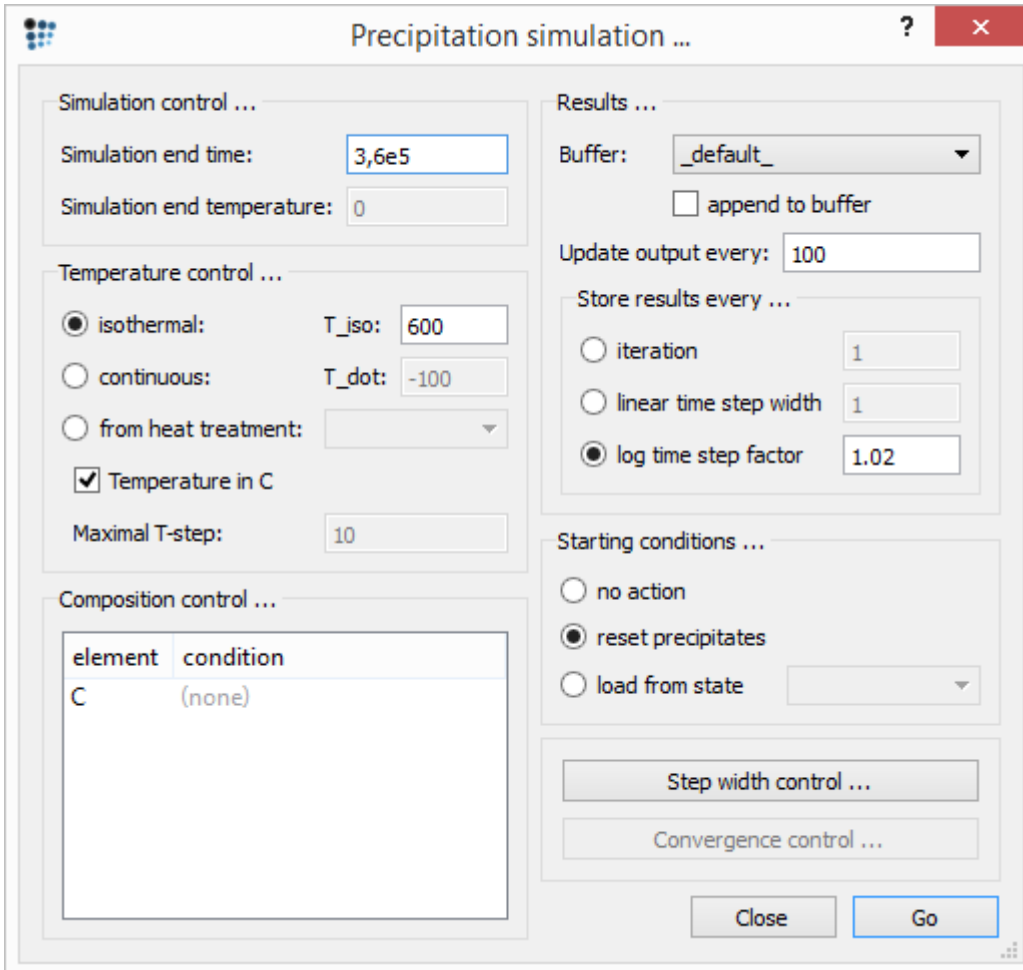
Both the histogram and the plot of phase fraction against time are updated during the calculation, so it is possible to follow the evolution of the size distribution and the phase fraction as the calculation takes place.

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 nucleation-density-increase-factor=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**'.



Precipitation simulation ...

Simulation control ...

Simulation end time:

Simulation end temperature:

Temperature control ...

☒ isothermal: T_iso:

☐ continuous: T_dot:

☐ from heat treatment:

☒ Temperature in C

Maximal T-step:

Composition control ...

element	condition
C	(none)

Results ...

Buffer:

☐ append to buffer

Update output every:

Store results every ...

☐ iteration

☐ linear time step width

☒ log time step factor

Starting conditions ...

☐ no action

☒ reset precipitates

☐ load from state

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=1,77e-010 (sve=1,77e-010), dcf=1, ro=1e+12, gsc=0 (dt=0, -/-
1)

FE +9.90768e-001(+0.00e+000) C +9.23192e-003(+0.00e+000)

-----

CEMENTITE_P0: FE75C25, nucl-site: d, nucl-dfm=6825,3, n_dot=0,0, ans=4e+021 (dt=0,
-/-1)

+ 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

ro - current dislocation density

gsc - number of grain classes used (meaningful for multi class grain growth model)

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

FE75C25 - composition of the most stable nuclei

nucl-site - nucleation sites

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

n_dot - nucleation rate

ans - available nucleation sites

- Last line:

+ nucleation of CEMENTITE_P0 started at 1.9531e-008 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) *****

900, recs=287; its=2/1, dt=0,0282379, time: 31,5719s (0,00877h), T=600 C (873,2 K), on Tue, 17:49:51

#Ferrite: BCC_A2, sv=1,77e-010 (sve=1,77e-010), dcf=0, ro=1e+012, gsc=0 (dt=0, -/-1)

FE +9,99771e-001 (+0,00e+000) C +2,28647e-004 (+0,00e+000)

-----

CEMENTITE_P0:      (250/..gs/1e+020/d)      f=0,03604/rm=4,07e-008/dfm=63,0,nuc1-dfm=63,2 (FE75C25)

FE74C25,  n_dot=0e+000 (ecdf=1),  ans=0,  mcomp(its:3),  step:  (dt=0,31,  rad-shrink/249)
```

- Additional information for the existing precipitate

(0/..gs/0e+00/d) - number of classes used / '+', '-' or '.', meaning: New class built, class deleted or no change; 'g' or 's' precipitate in classes are growing or shrinking / number of precipitates / nucleation sites

f - mole fraction of precipitate phase

rm - mean radius of precipitate phase

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

dt - maximum time step allowed due to the precipitate condition

The carbon content of the matrix has decreased from 9.2×10^{-3} initially (iteration 1) to 2.3×10^{-4} in iteration 900. The precipitate phase uses **250** classes and consists of roughly 1×10^{20} particles. The mole fraction of cementite in the matrix is **0.03604** (3.6%). There is a small positive driving force for nucleation (**63 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 **0,31 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_PO versus time. Drag and drop **NUM_PREC\$CEMENTITE_PO** (number of cementite precipitates) into the first of these, **NUCL_RATE\$CEMENTITE_PO** (nucleation rate) into the second. In the third, add **R_MEAN\$CEMENTITE_PO** (mean radius), **R_CRIT\$CEMENTITE_PO** (critical radius), **R_MIN\$CEMENTITE_PO** (minimum radius) and **R_MAX\$CEMENTITE_PO** (maximum radius). These variables can be found under '**kinetics: precipitates**' and '**kinetics: nucleation**' in the '**variables**' window.

Type in the following settings for the plots:

1. Plot 1

- Title: '**Phase fraction of cementite precipitate**'
- Y-axis title: '**Phase fraction**'

2. Plot 2

- Title: '**Number of precipitates**'
- Y-axis title: '**Number of precipitates [10^{20} m^{-3}]**'
- Y-axis factor: '**1e-20**'

3. Plot 3

- Title: '**Nucleation rate**'
- Y-axis title: '**Nucleation rate [$10^{26} \text{ m}^{-3} \text{ s}^{-1}$]**'
- Y-axis factor: '**1e-26**'

4. Plot 4

- Title: '**Precipitate radius**'
- Y-axis title: '**Precipitate radius [μm]**'
- Y-axis type: '**log**'
- Y-axis factor: '**1e6**'

5. Default x-axis

- Use for all plots: **yes** - Title: '**Time [h]**'
- Type: '**log**'
- Scaling: '**1e-12..**'
- Factor: '**1/3600**'

Note the usage of the html-tags for the text with special features:

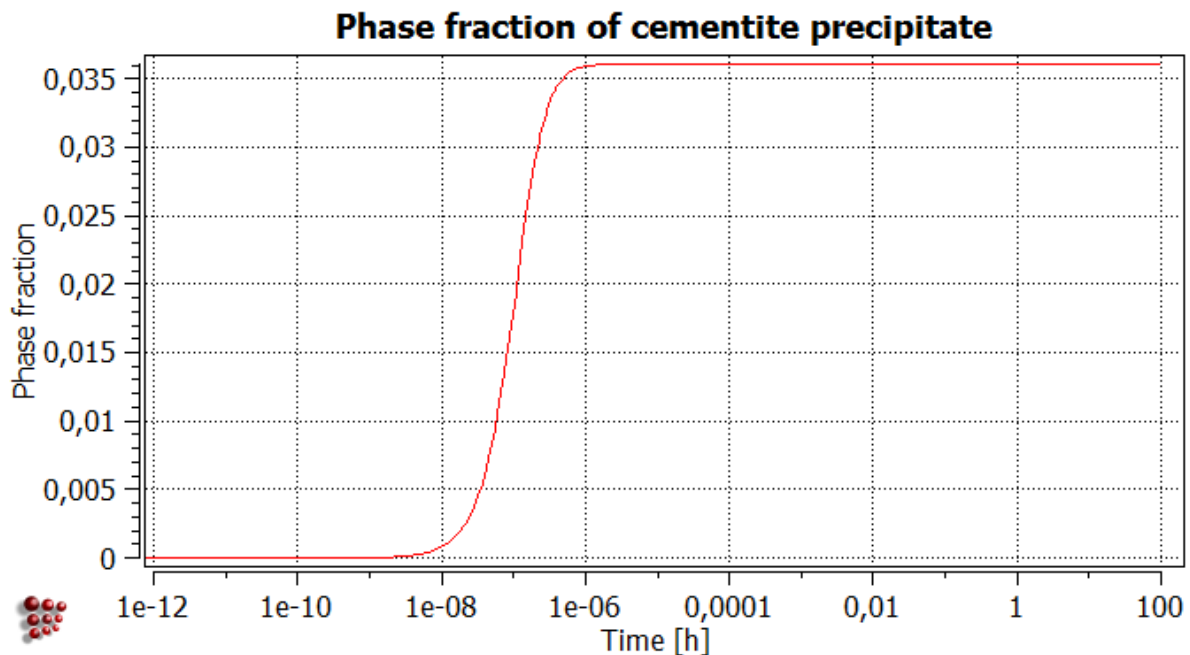
- the text between the '^{' and '}' tags will be displayed as superscript (e.g. **10²⁰** appears as **10²⁰**)

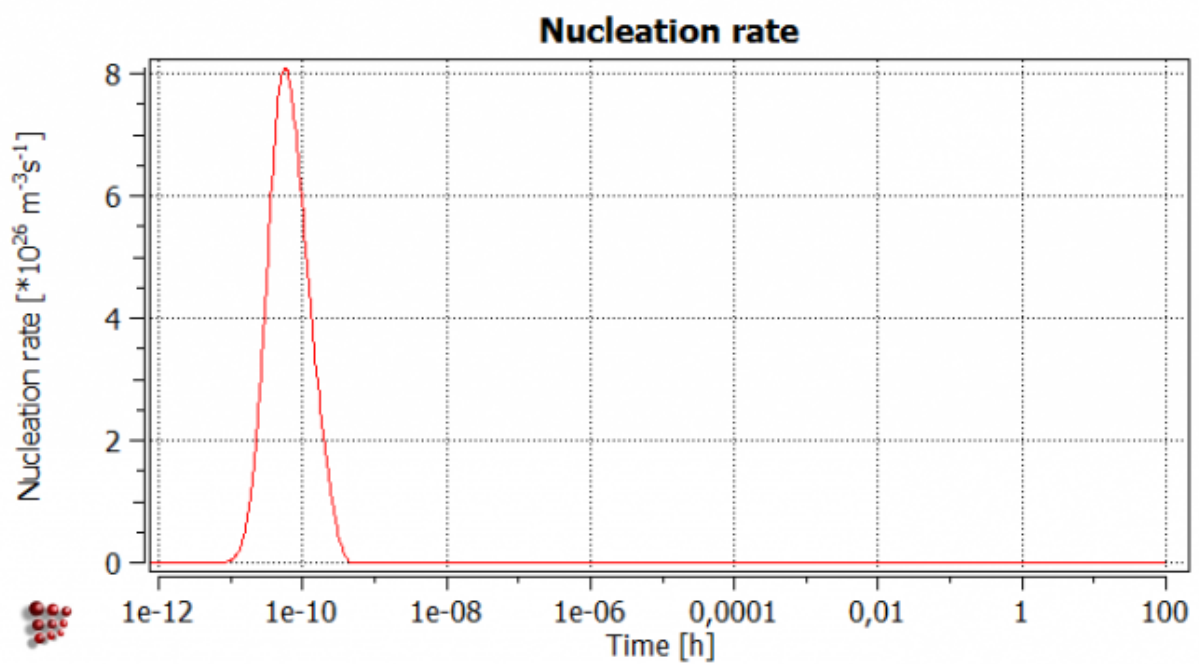
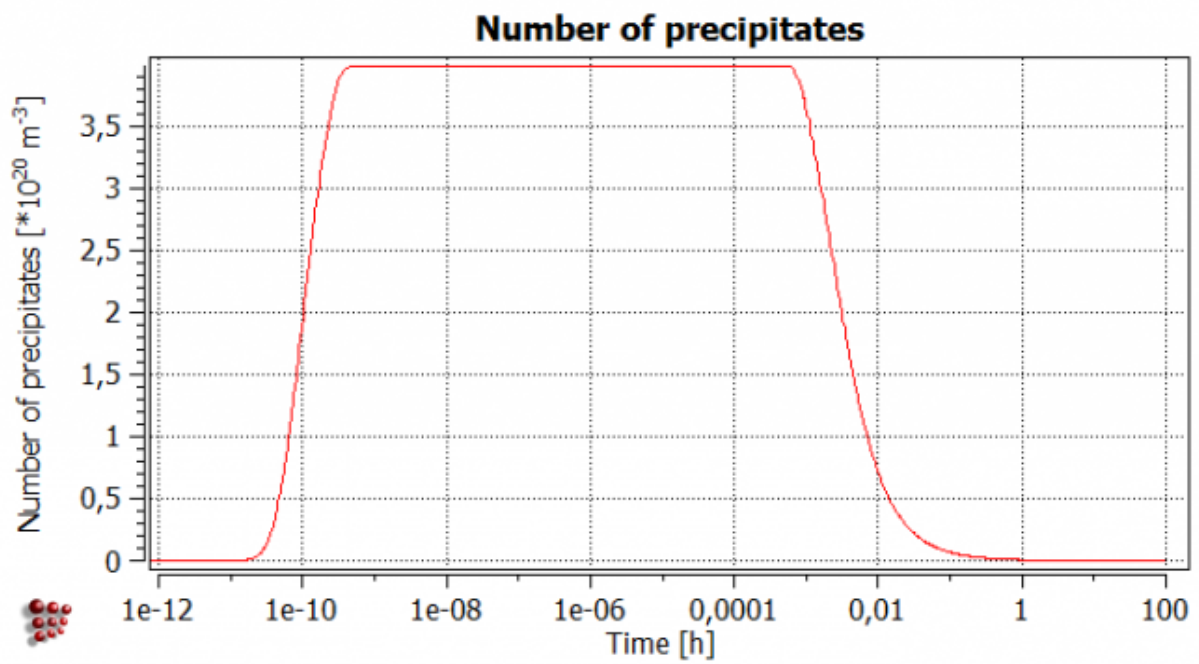
- '<html>μ</html>' is used to display the Greek letter μ

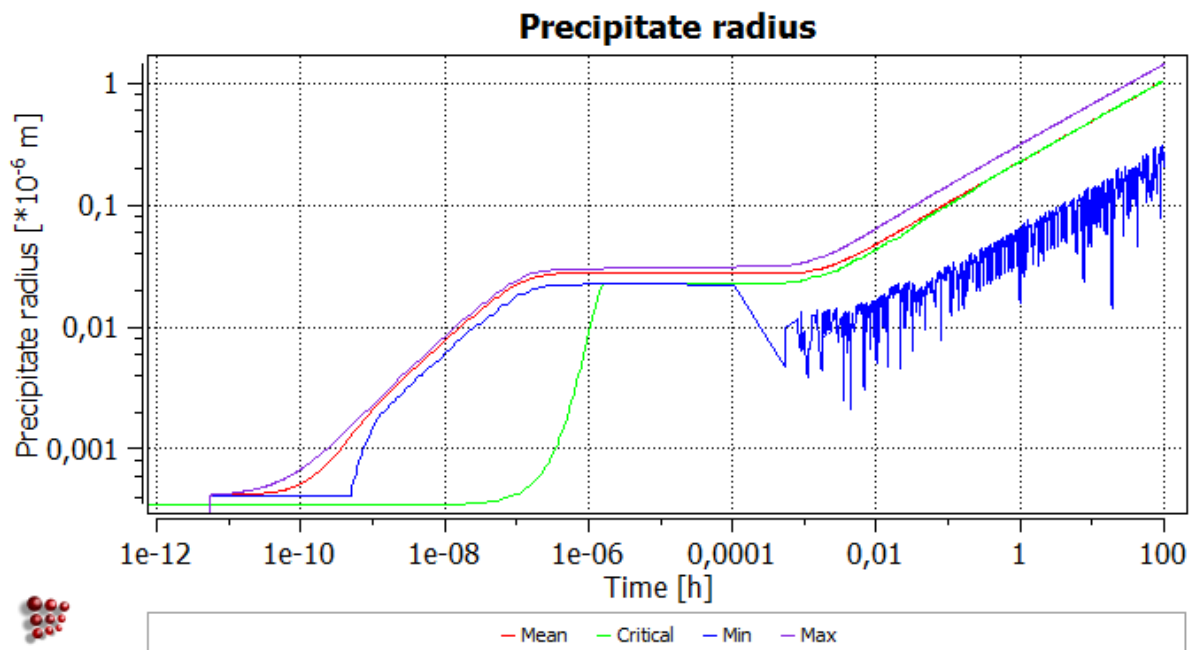
Using these plots, the different stages of nucleation, growth and coarsening can be identified. During the **nucleation** stage, between $1\text{e-}11$ and $1\text{e-}9$ hours, the number of precipitates increases rapidly, but since these precipitates are, as yet, extremely small, the phase fraction 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 $1\text{e-}9$ to $1\text{e-}6$ 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 $1\text{e-}3$ 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).

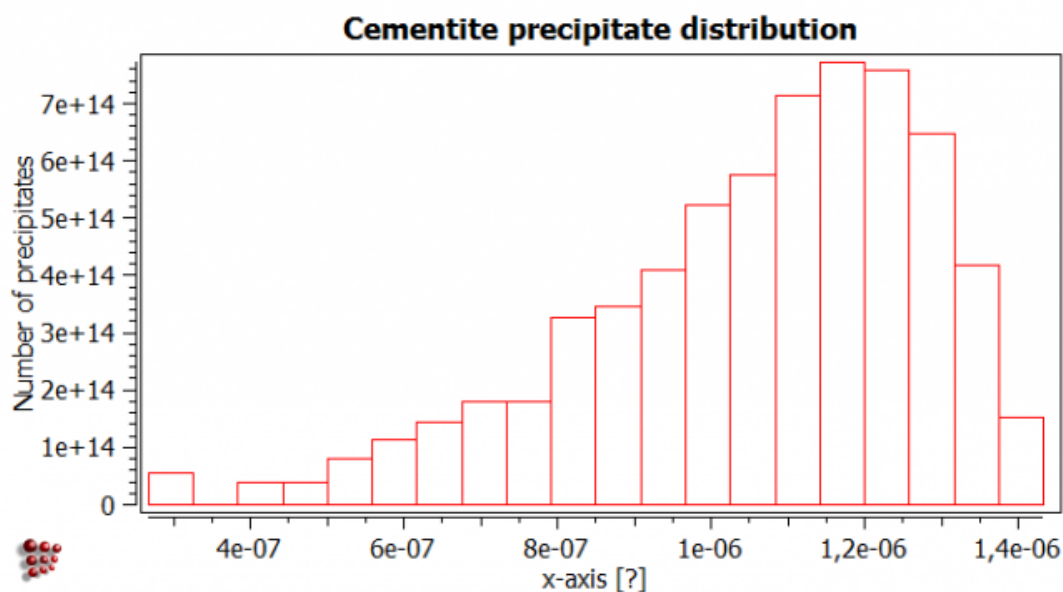






HISTOGRAMS OF PRECIPITATE SIZE DISTRIBUTION

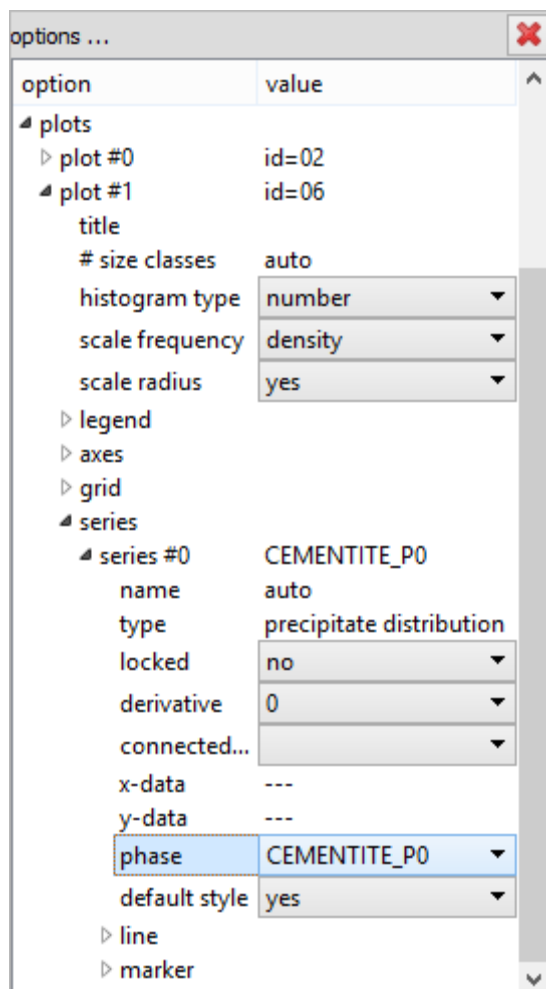
The plot above shows only the variation of the mean radius with time, but more detailed information on the distribution of particle sizes can be found on the histogram. At the end of the calculation, the final size distribution is shown on the histogram. The distribution at other stages of the calculation 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.



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:

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

In the histogram window, create a new plot and add a new series for it (set '**CEMENTITE_P0**' for '**phase**'). 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.



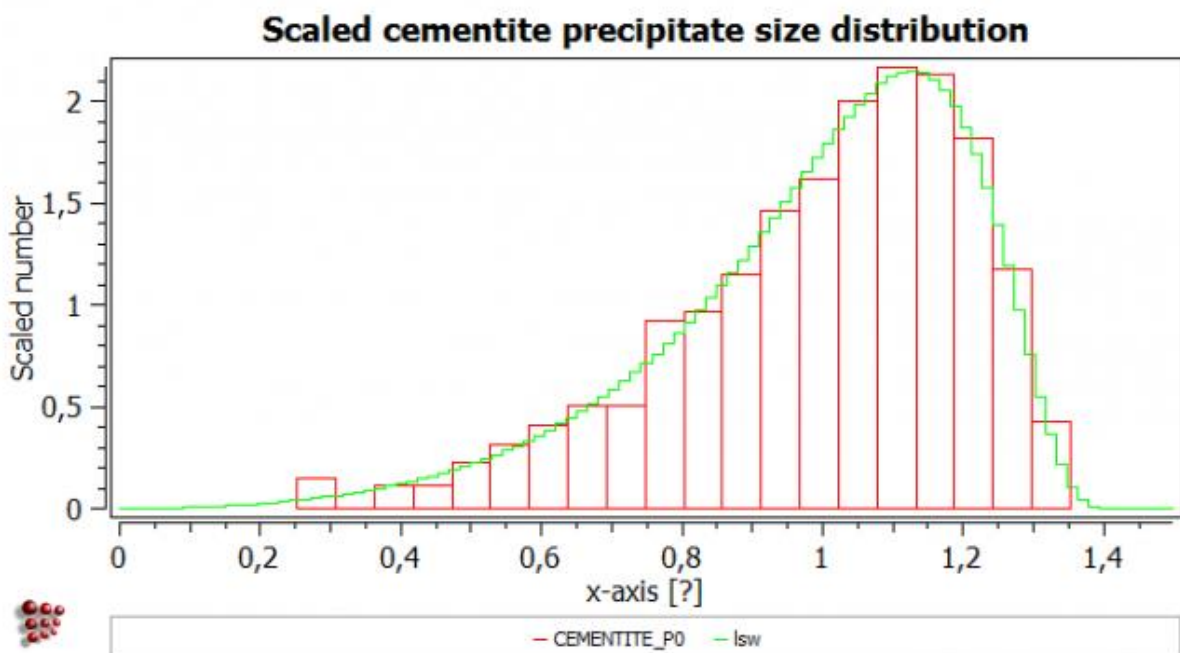
Enter the LSW function, either using the '**Functions and Variables**' box or by using the following command-line in the console:

```
set-function-expression function=lsw expression= $x^2 \cdot (3/(3+x))^{(7/3)} \cdot ((3/2)/(3/2-x))^{(11/3)} \cdot \exp(-x/(3/2-x)) \cdot 4/9$ 
```

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.



T15: EFFECT OF MICROSTRUCTURE AND CONDITIONS (PART 1)

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

database: mc_fe.tdb; mc_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.

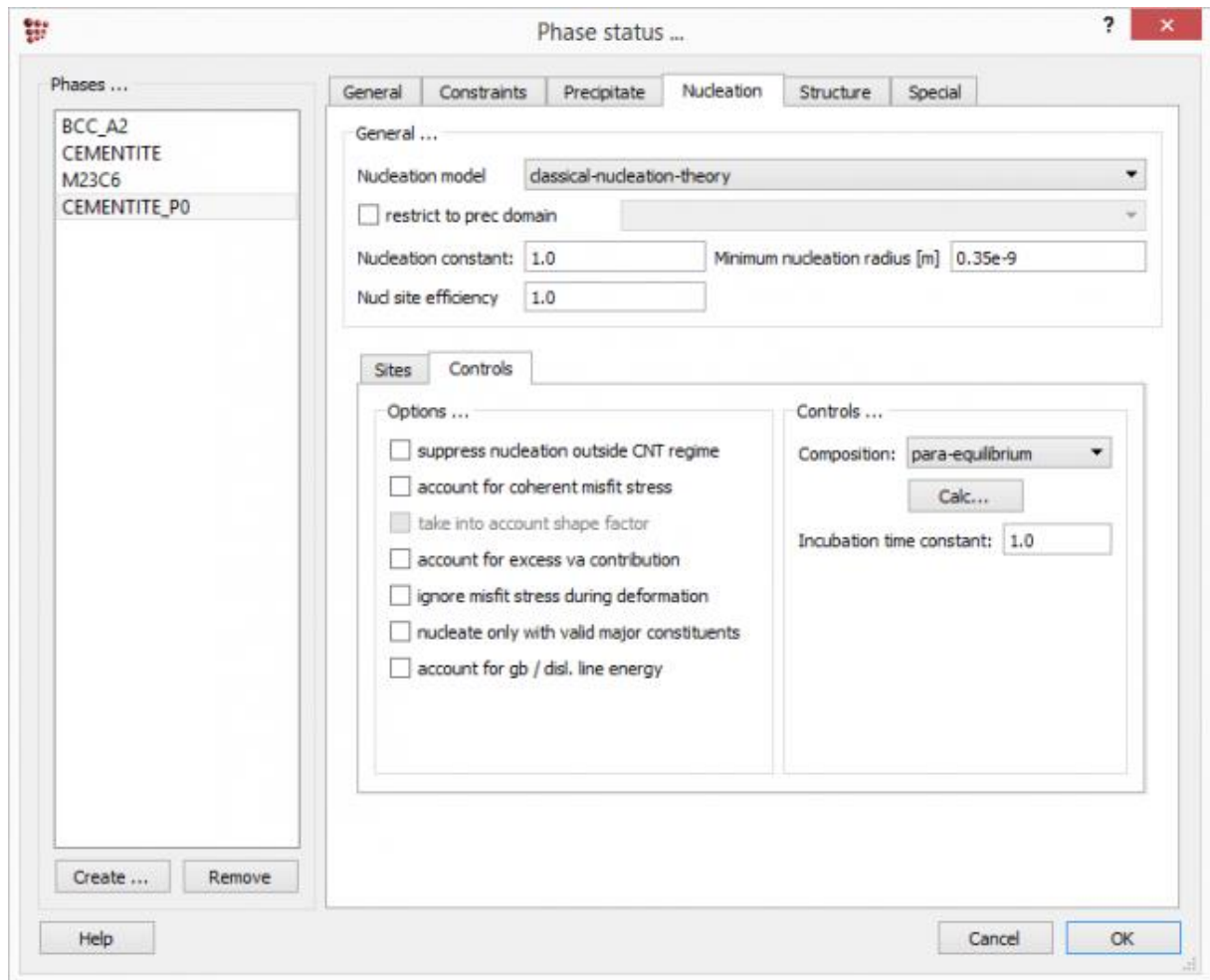
Calculate an equilibrium at 600°C and observe the contents of the '**Phase summary**' window. It can be seen that M₂₃C₆ is the stable phase at equilibrium. However, it is known from experience that the first phase to form on heat-treatment is cementite. Go to '**Global > Phase status**', suspend the '**M₂₃C₆**' phase and calculate an equilibrium once again 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 89.9 % Fe. This high amount of Cr is rather unusual for cementite, as it is expected to be rather Fe-rich. Hence, Fe is set as the major constituent for this carbide. However, MatCalc detects that the Cr-content in cementite is greater than the one of the major constituent for this phase (Fe) and a '***maj*!**' warning flag appears in the 'phase summary' window.

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 M₂₃C₆.

NUCLEATION MODEL FOR CEMENTITE

SETTING UP THE SIMULATION

Create a precipitate phase **CEMENTITE_P0**, using '**Global > Phase status**'. 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 '**Nucleation > 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. 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_PREC\$CEMENTITE_P0** (found under '**kinetics: precipitates**')

2. **XPR\$CEMENTITE_PO\$CR** (Cr content of the cementite precipitate phase) and **X_NUCL\$CEMENTITE_PO\$CR** (Cr content of the nucleus). The latter can be found under '**kinetics: nucleation**'.
3. **X\$BCC_A2\$C** (carbon content of BCC matrix)
4. **NUM_PREC\$CEMENTITE_PO** (found under '**kinetics: precipitates**')
5. **R_MEAN\$CEMENTITE_PO** (found under '**kinetics: precipitates**')

Label the y-axes as follows

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

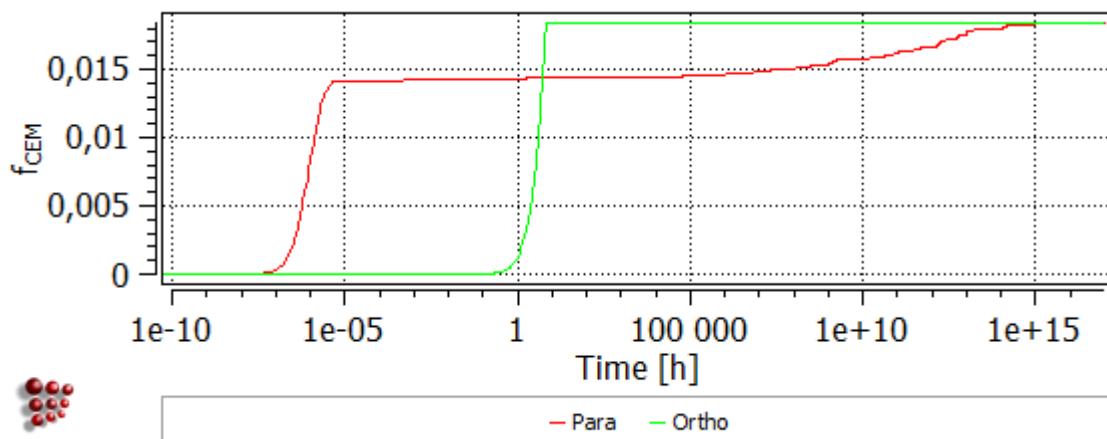
Save the workspace.

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_PO 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**".

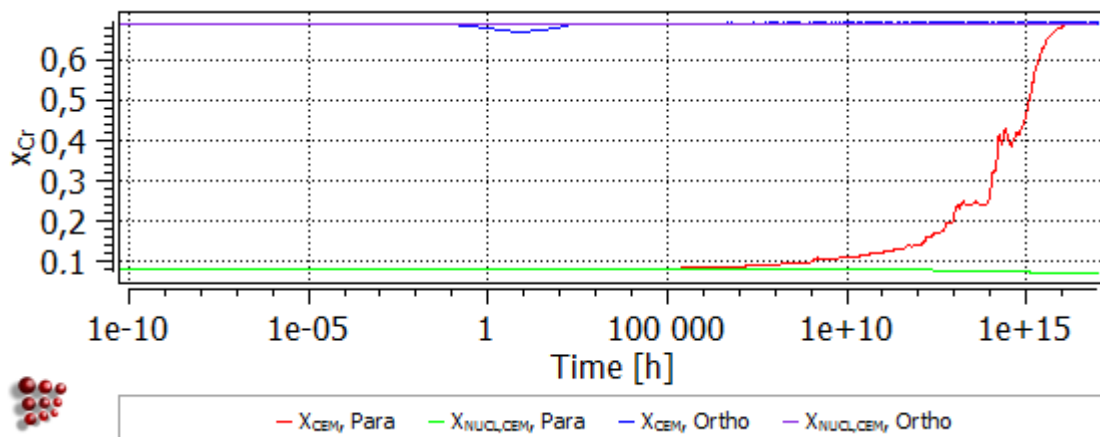
INTERPRETATION OF RESULTS

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.

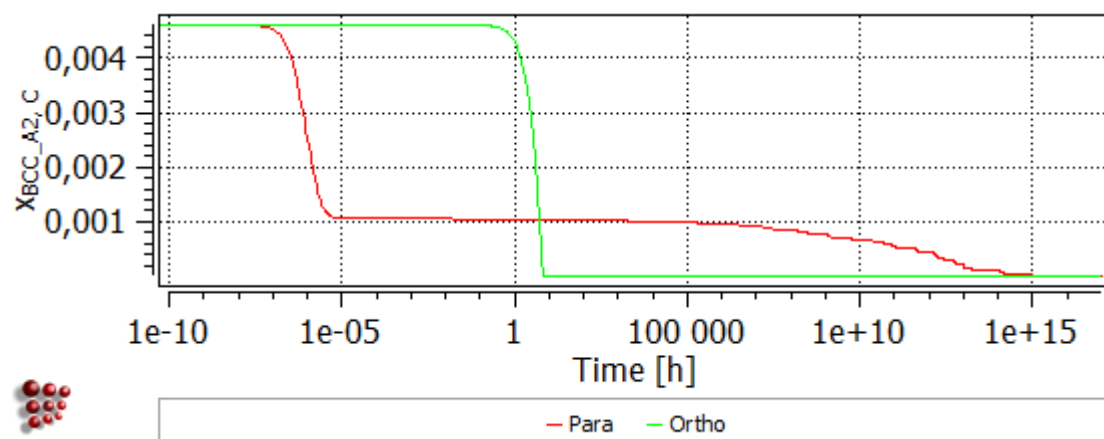


The para-equilibrium model stipulates that the Cr content of the nuclei ($X_{NUCL,CEM, Para}$) be equal to that of the matrix. This decreases towards longer times at temperature, as the matrix becomes depleted in Cr. This depletion is caused by the Cr-enrichment of the precipitates by diffusion; their Cr content ($X_{CEM, Para}$) increases up to the equilibrium value of around 0.69 (mol. fr.).

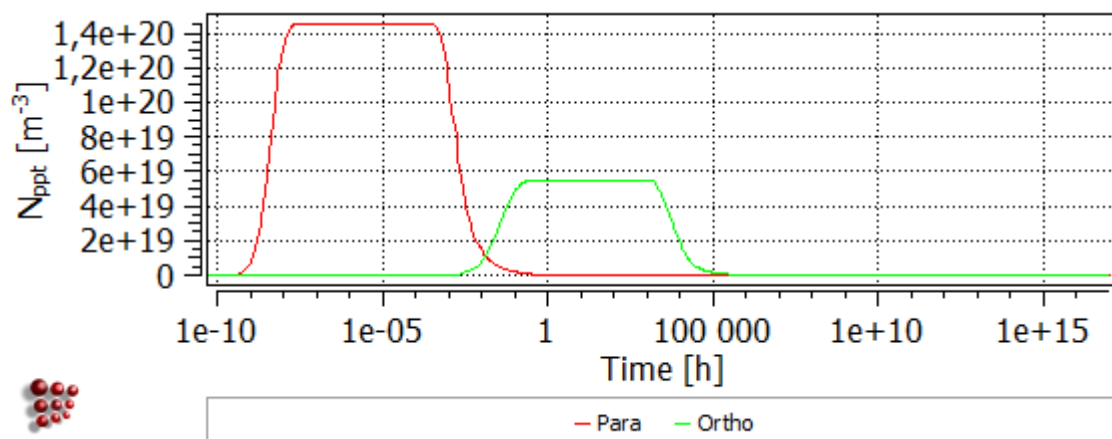
In the ortho-equilibrium case, the cementite nucleates with its equilibrium Cr content, and there is little or no change in the Cr content of the precipitates during the heat-treatment. It is this requirement for full equilibrium which accounts for the long incubation time for cementite when the ortho-equilibrium model is used; the formation of a critical nucleus with ortho-equilibrium composition requires the (slower) diffusion of Cr.



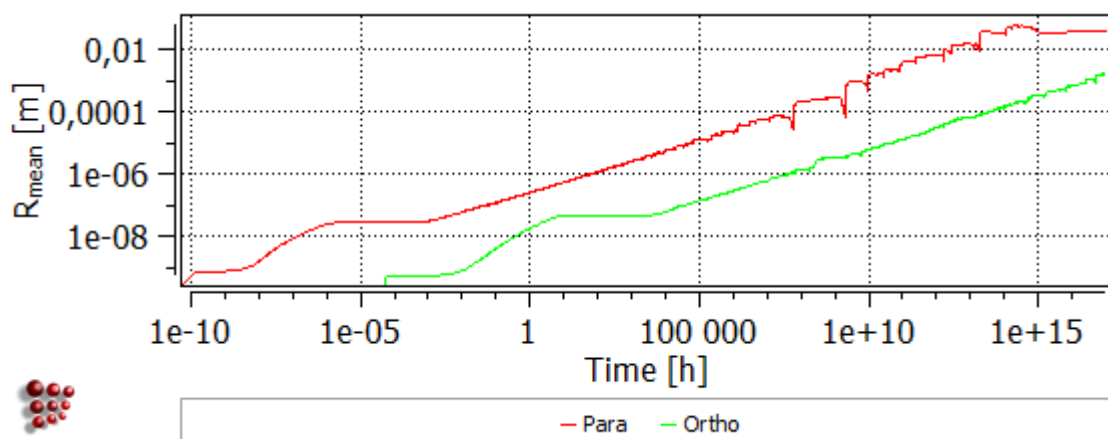
In the plot of $X_{BCC_A2\%C}$ (the carbon content of the BCC matrix), it can be seen that the depletion of the matrix in carbon exactly follows the increase in precipitate fraction for both models.



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:



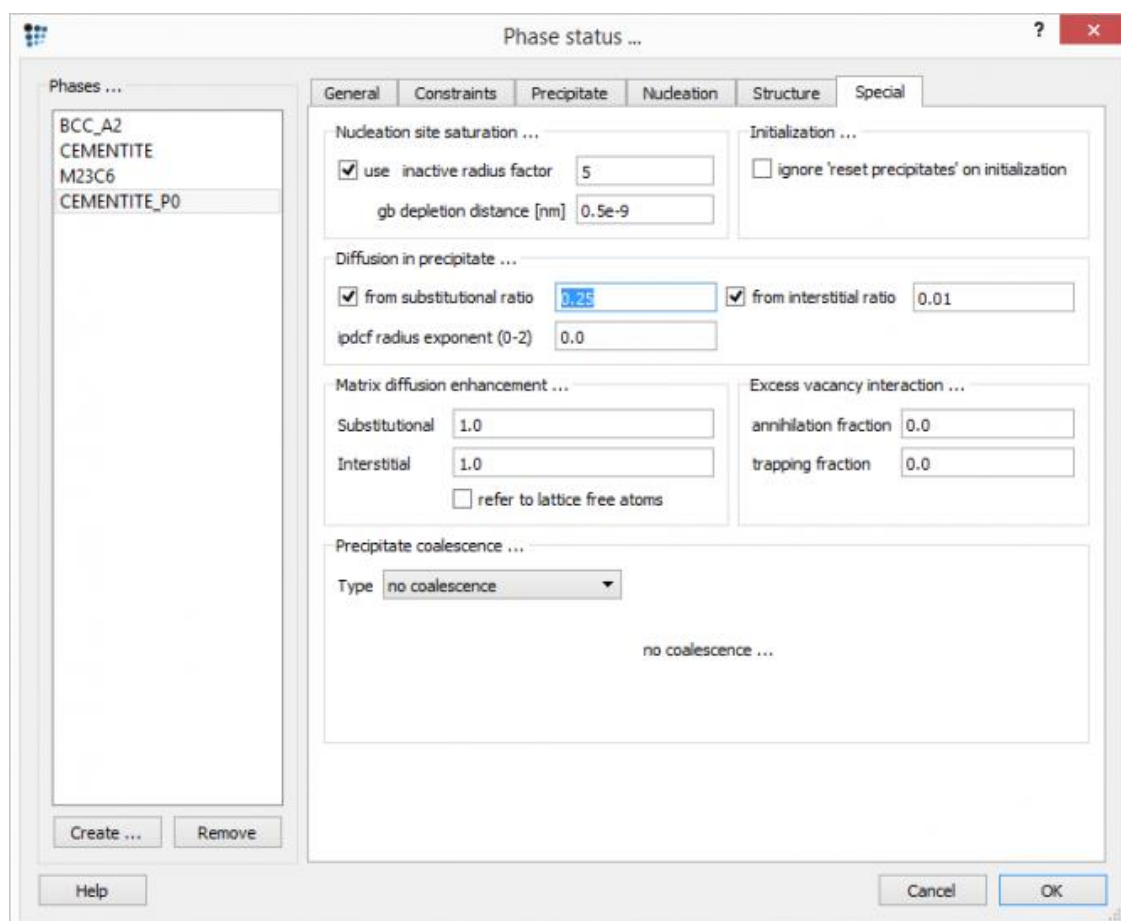
The use of the para-equilibrium nucleation model gives better qualitative agreement with experimental observations of the rapid precipitation of cementite at temperatures such as 600°C in alloy steels. An example in the [Examples](#) section, in which this issue is considered in more detail, will be available shortly.

DIFFUSIVITY IN PRECIPITATES

SETUP

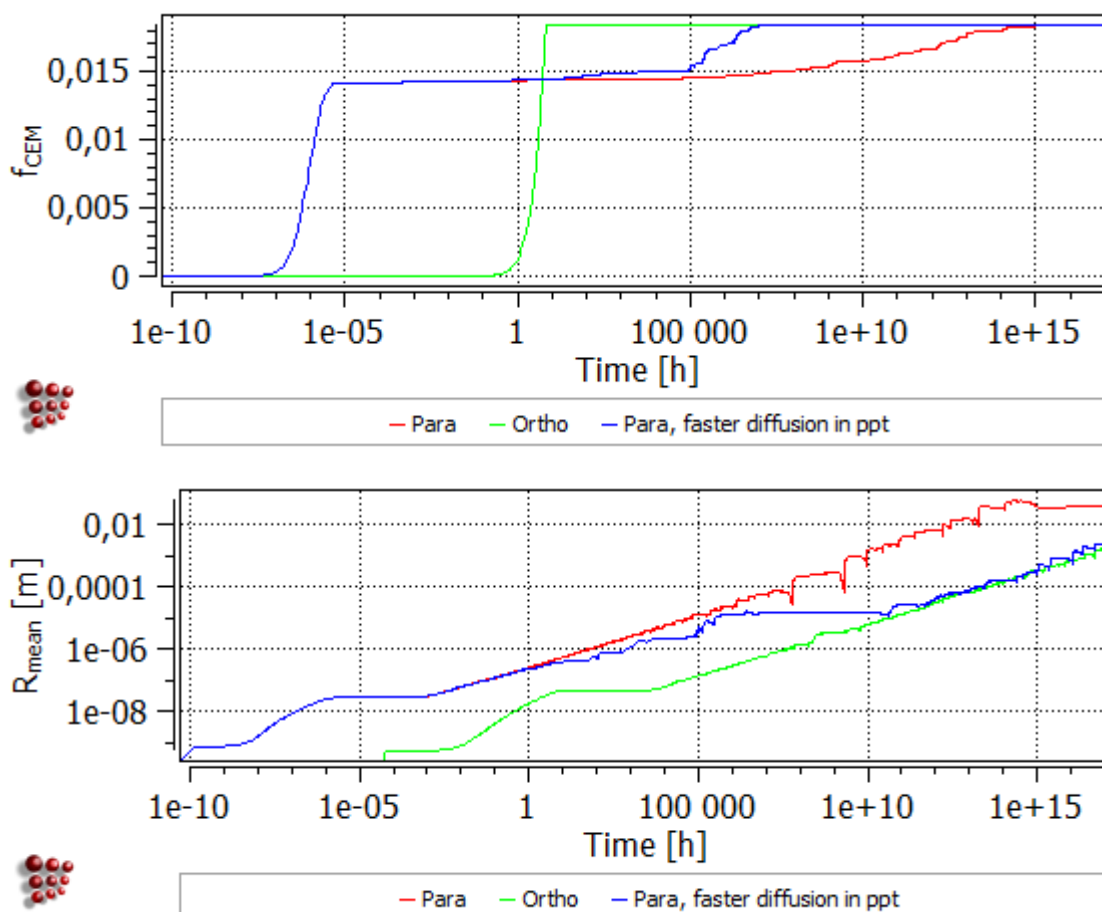
It was seen above that, using the para-equilibrium model, cementite precipitates formed with a Fe-rich composition and subsequently enriched in Cr. The rate of enrichment depends on the ease with which chromium can diffuse into existing precipitates.

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.

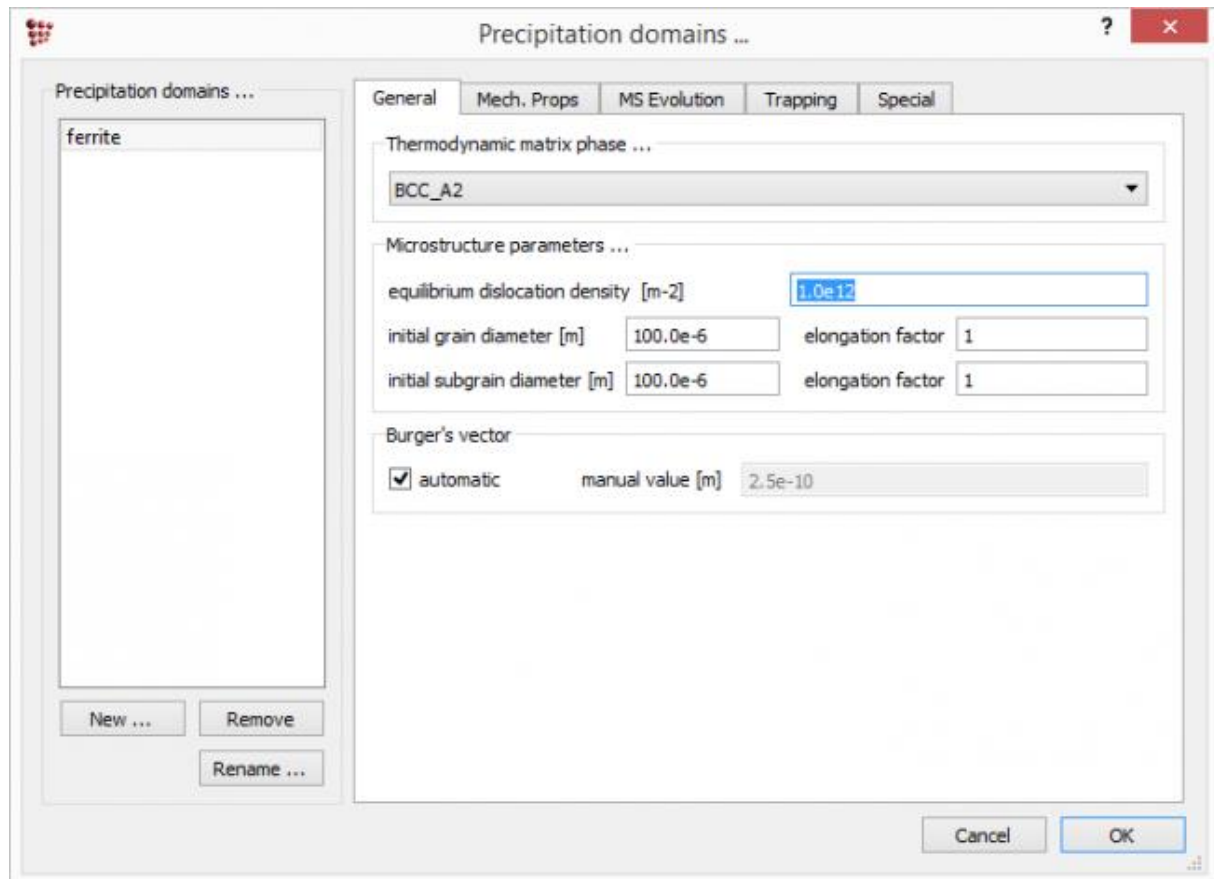


MICROSTRUCTURAL PARAMETERS AND NUCLEATION SITES

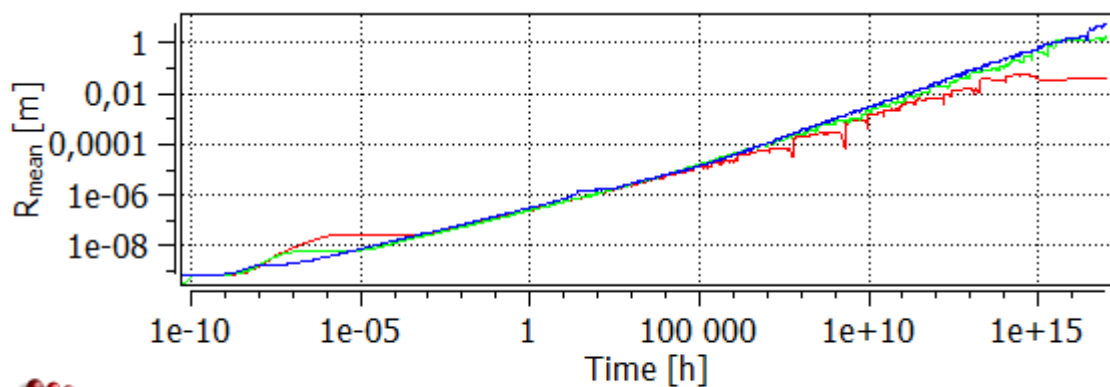
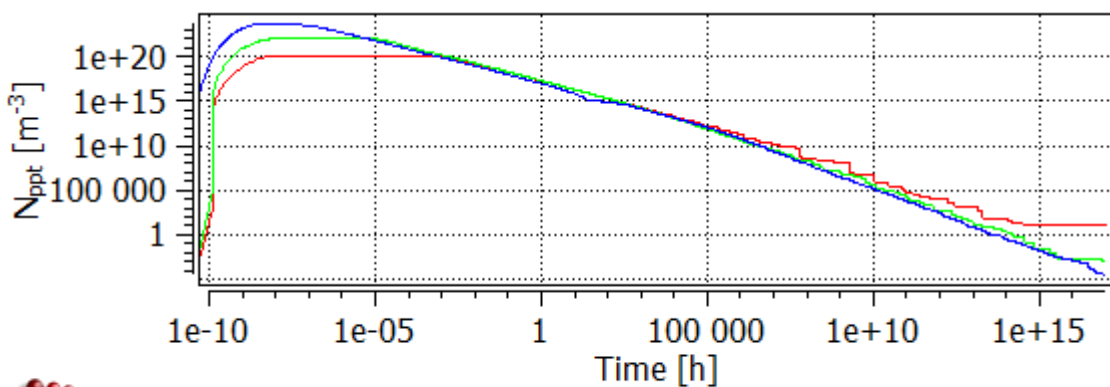
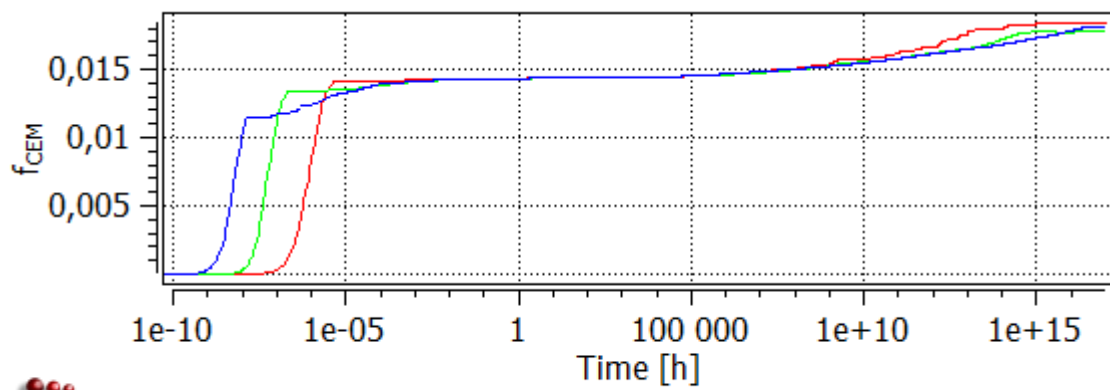
SETUP

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 > General**'. It contains a few data on the microstructure like dislocation density or grain diameter. 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.

T16: EFFECT OF MICROSTRUCTURE AND CONDITIONS (PART 2)

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

database: mc_fe.tdb; mc_fe.ddb

CONTENTS

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

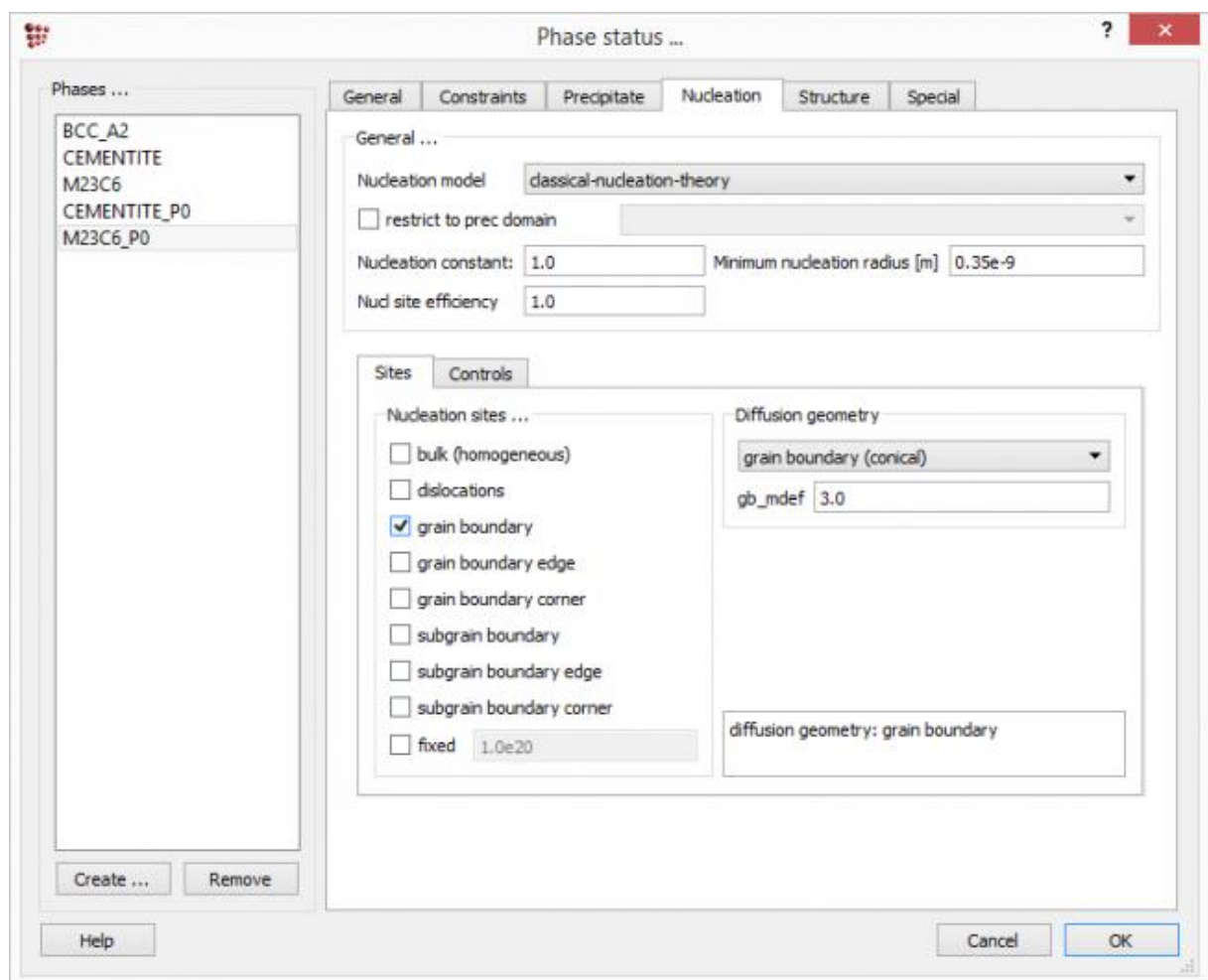
BEFORE STARTING...

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 '**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 > General**', 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:

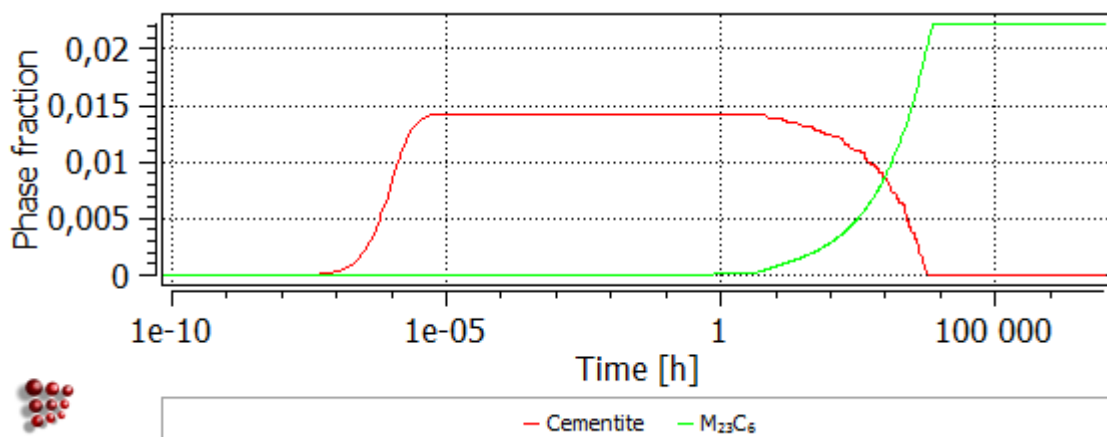
1. **F\$CEMENTITE_P0, F\$M23C6_P0** (fraction of cementite and M23C6 precipitated, respectively)

2. **XPR\$CEMENTITE_P0\$CR, X\$BCC_A2\$CR** (Cr content of cementite precipitates and matrix, respectively)
3. **X\$BCC_A2\$C** (C content of matrix)
4. **NUM_PREC\$CEMENTITE_P0, NUM_PREC\$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)

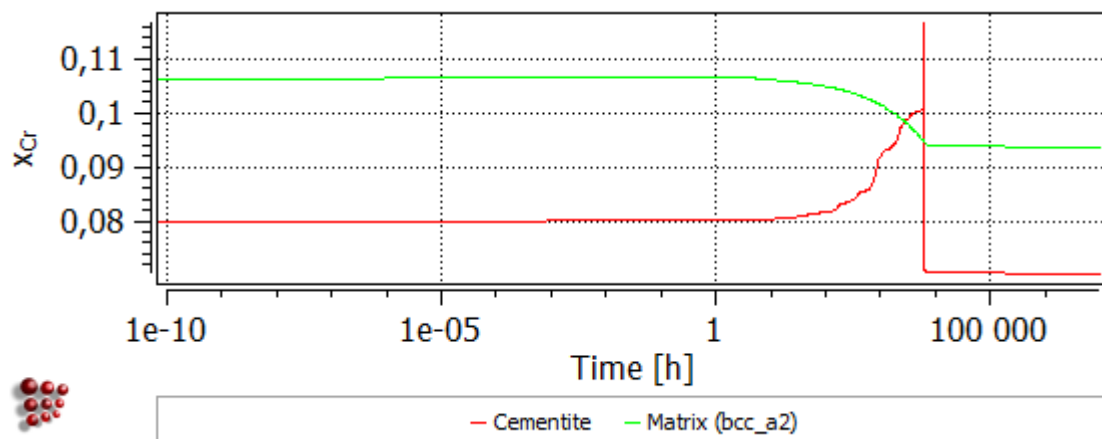
Run the kinetic simulation, with an isothermal heat treatment at **600°C** as before, and an end time of **3.6e+10 s**.

INTERPRETATION OF RESULTS

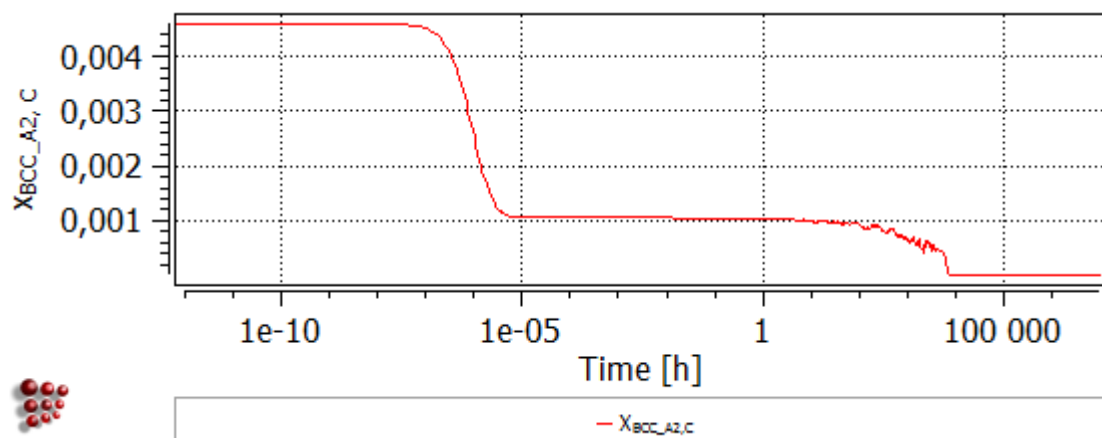
Plot 1: Cementite appears rapidly and reaches a steady-state precipitate fraction. M₂₃C₆ starts to form after around 1 hour at 600°C; this is at the expense of cementite, which redissolves. By the end of the simulation, all the cementite has dissolved and M₂₃C₆ has reached its equilibrium phase fraction.



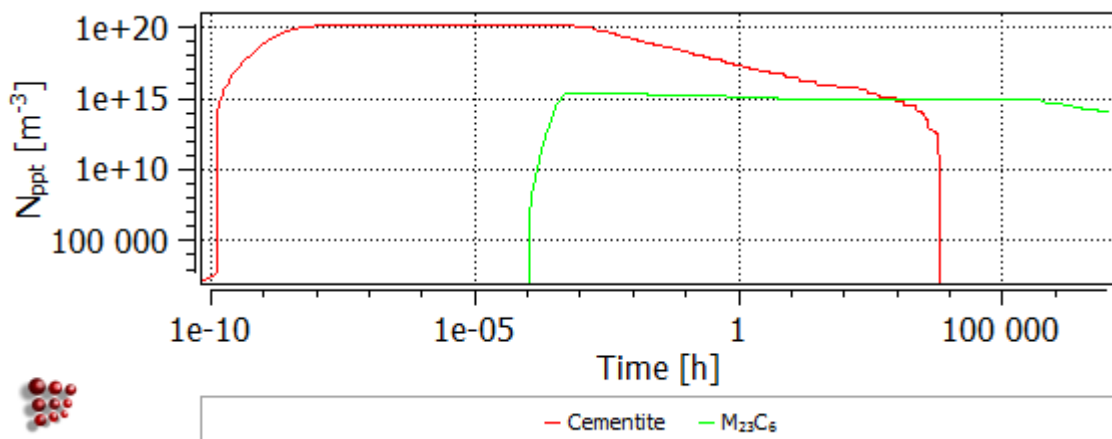
Plot 2: This shows that cementite enrichment has started in the time of the cementite dissolution.



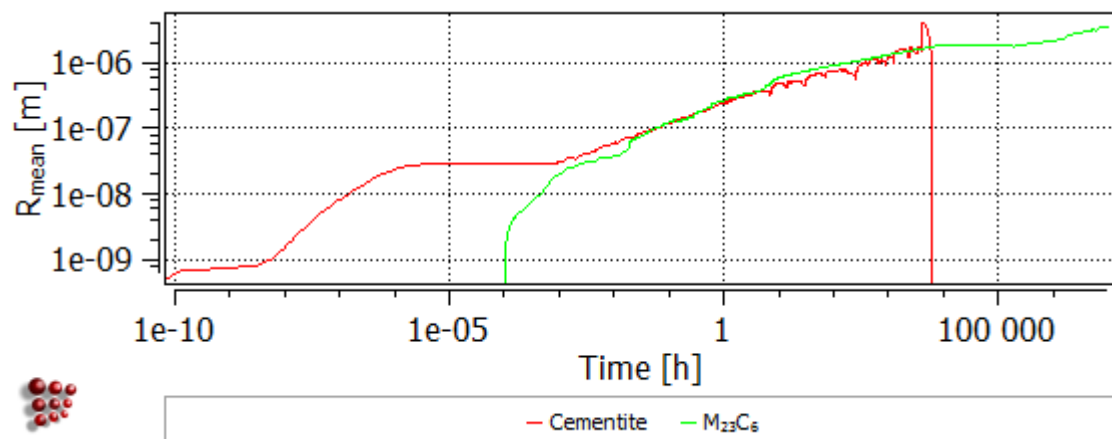
Plot 3: The depletion of the matrix in carbon occurs in two stages. The first of these corresponds to the formation of cementite, and the second to the formation of $M_{23}C_6$.



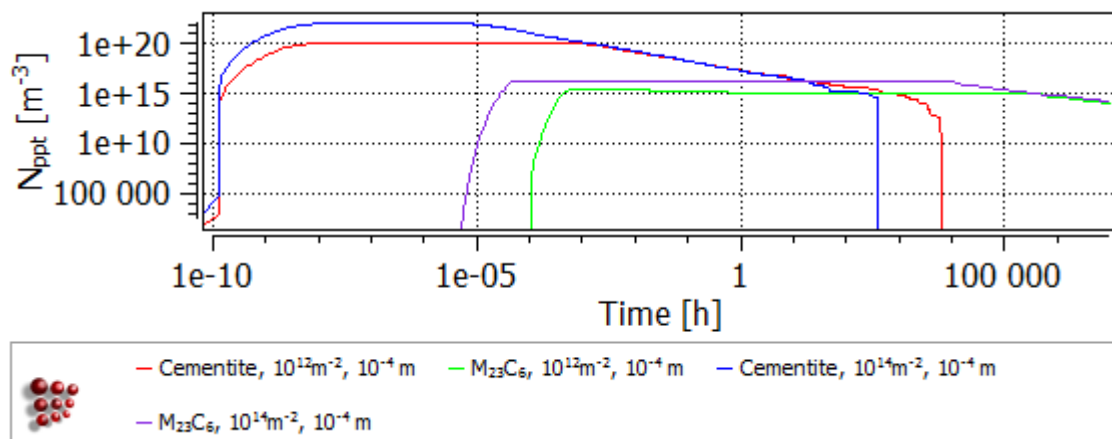
Plot 4: The number of $M_{23}C_6$ precipitates is lower than the one cementite precipitates which is due to the lower amount of the nucleation sites - there are less sites on the grain boundaries than on the dislocations. The reduction in the number of cementite precipitates is both due to the coarsening 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.



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.

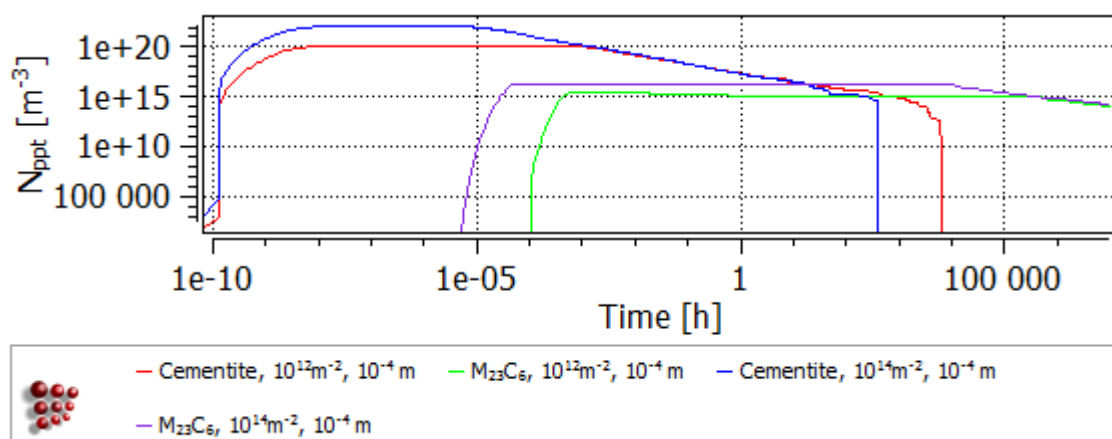


EFFECT OF DISLOCATION DENSITY

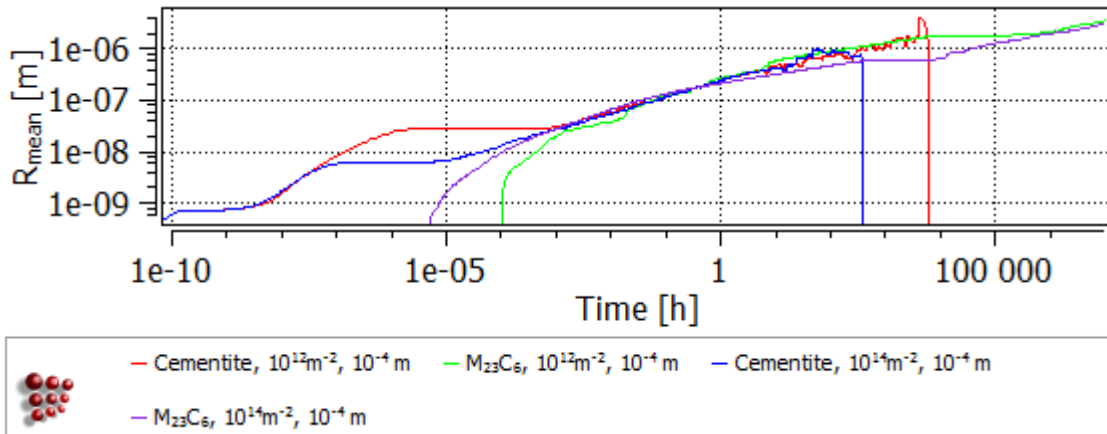
Duplicate and lock the series and re-run the simulation with a dislocation density of **$1e14 m^{-2}$** , leaving the grain size the same.

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.

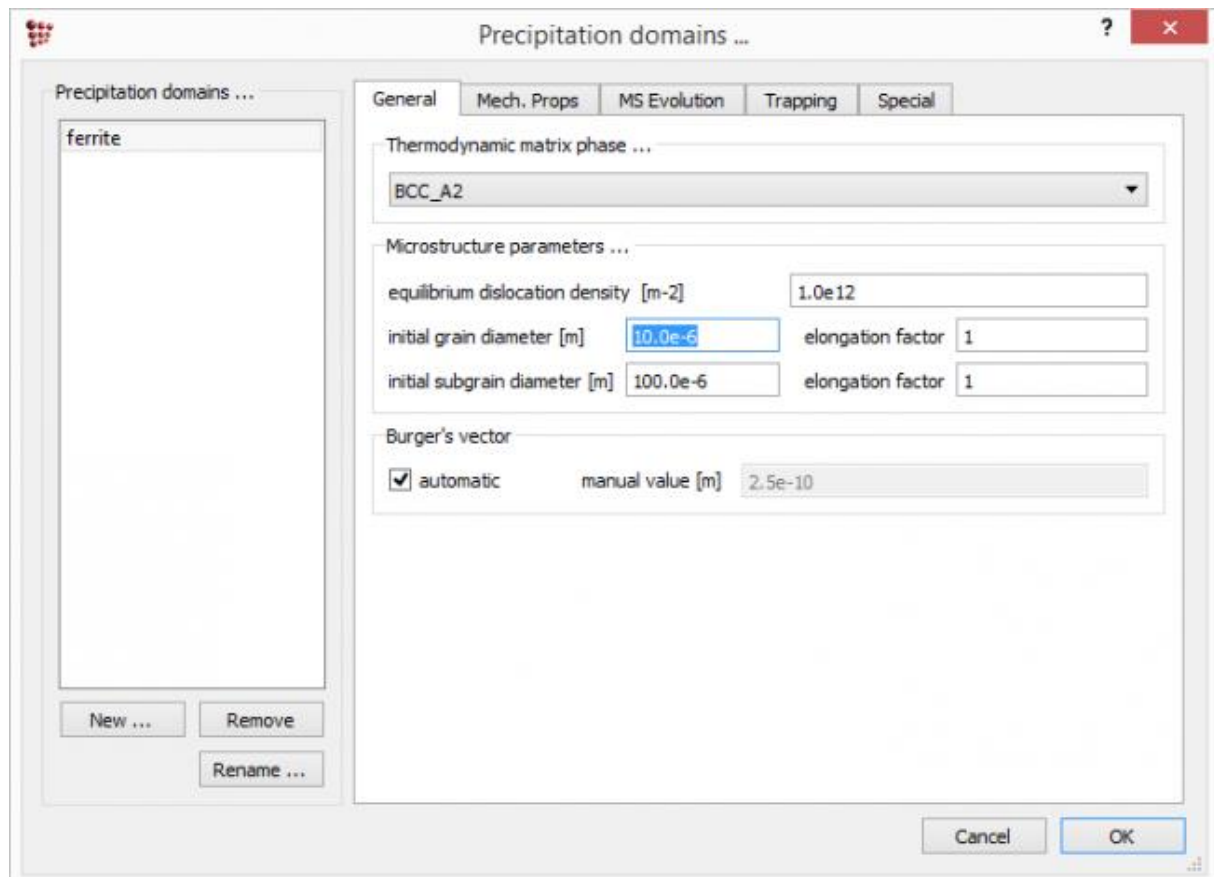


With a higher dislocation density, the cementite particles do not become so large during the growth stage. However, coarsening begins earlier, and the curve of radius versus time for the coarsening precipitates eventually becomes parallel with that for the lower dislocation density.



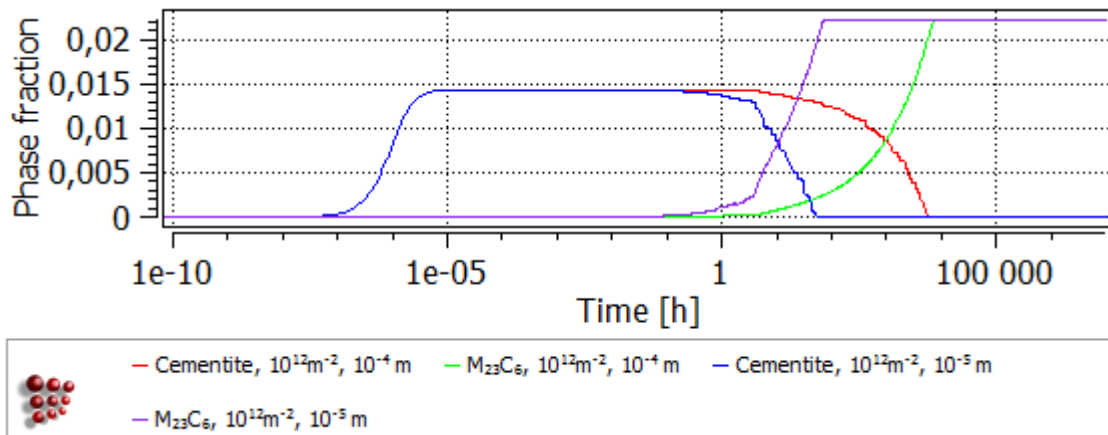
EFFECT OF GRAIN DIAMETER

Reopen '**Global > Precipitation domains > General**'. Reset the dislocation density to **$1\text{e}12\text{ m}^{-2}$** , set the grain diameter to **$10\text{e}-6\text{ m}$** and re-run the simulation.

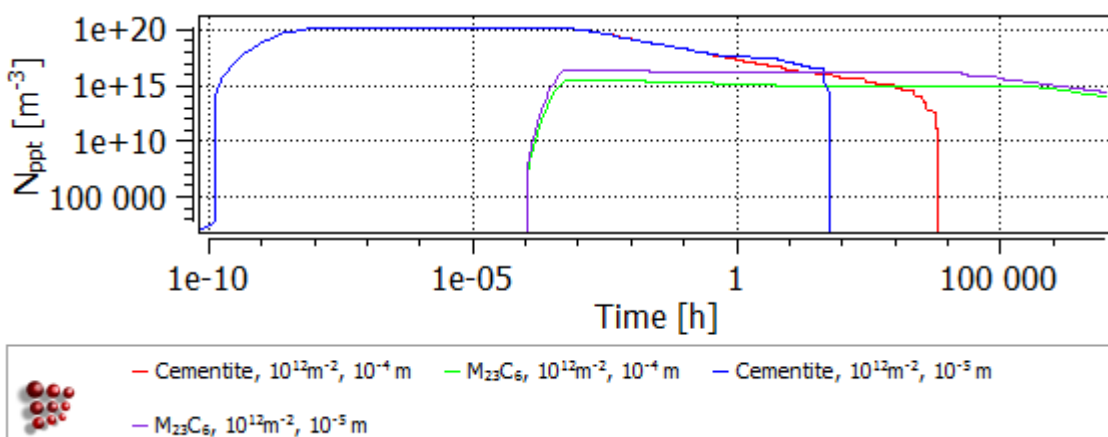


RESULTS:

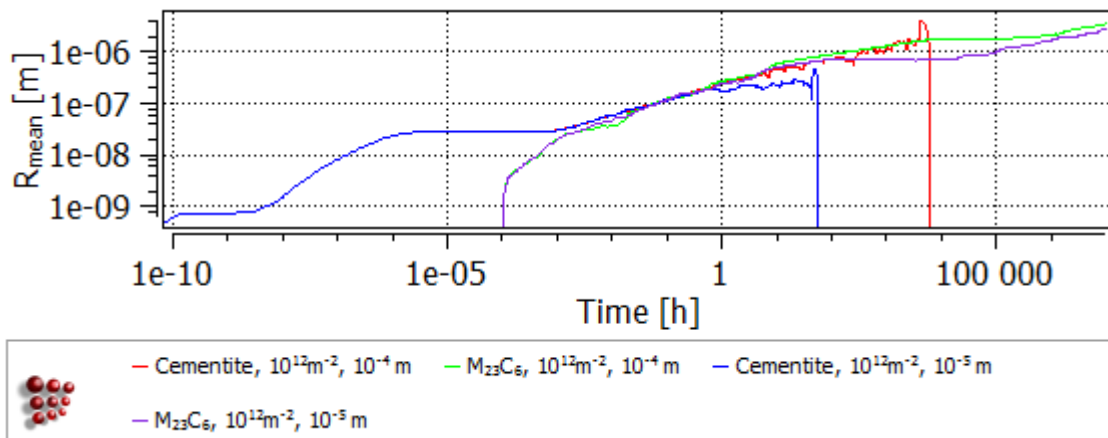
As might be expected, reducing the grain diameter accelerates the precipitation kinetics of $M_{23}C_6$, by providing more nucleation sites. It also accelerates the dissolution of cementite, which begins to dissolve when $M_{23}C_6$ starts to precipitate.



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.



T17: COMPLEX MULTI-STAGE HEAT TREATMENTS

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

database: mc_fe.tdb; mc_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

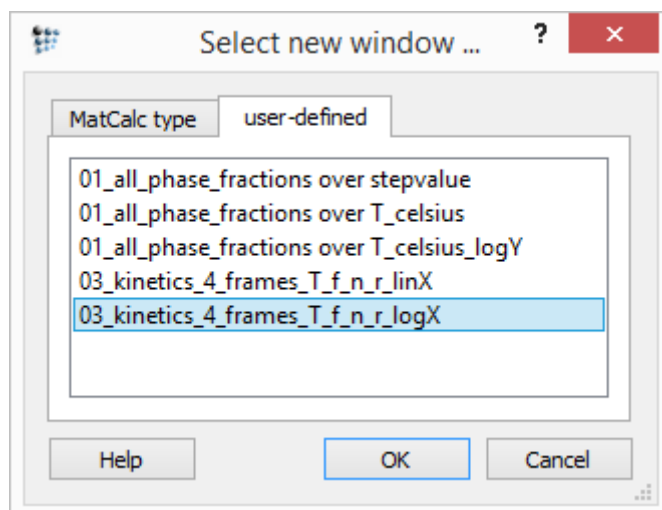
SETTING UP GUI, THERMODYNAMICS, PRECIPITATES AND PRECIPITATION DOMAINS

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. Leave all the other settings at their default values. Read in the mobility data.

SETUP GUI

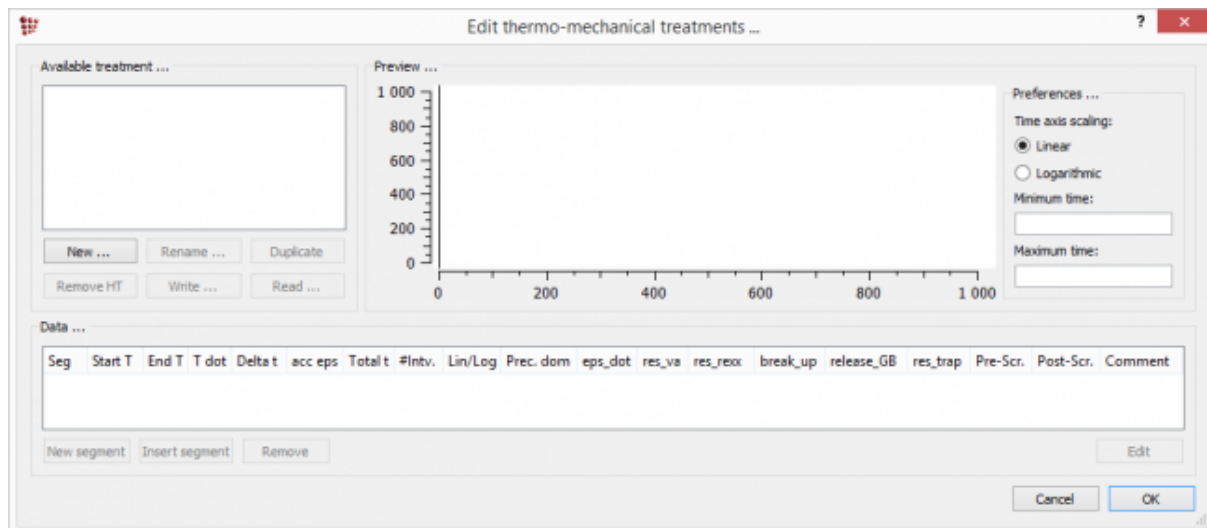
In order to follow the precipitation kinetics simulation results, usually the plots for phase fraction, precipitation number density and mean radius are in the scope of interest. In cases of complex heat-treatments, a plot of the system temperature during the process time is also needed. Of course, these plots can be prepared manually by user, as done in the previous tutorials. However, due to the frequent need for these 4 plots, an automatic script preparing those is included in MatCalc. In order to use it, go to '**View**' > '**Create new window**' and switch to the '**user-defined**' tab. Click on '**03_kinetics_4_frames_T_f_n_r_logX**' to open a window with those four plots already set.



Use a default x-axis and set the axis type to 'log'. Scale from '10..'. The axis title is 'time / s'.

DEFINITION OF THE HEAT TREATMENT

Open '**Global > Thermo-mech. treatments ...**'. This dialog represents a very useful editor for definition of complex process treatments by a sequence of linear segments.

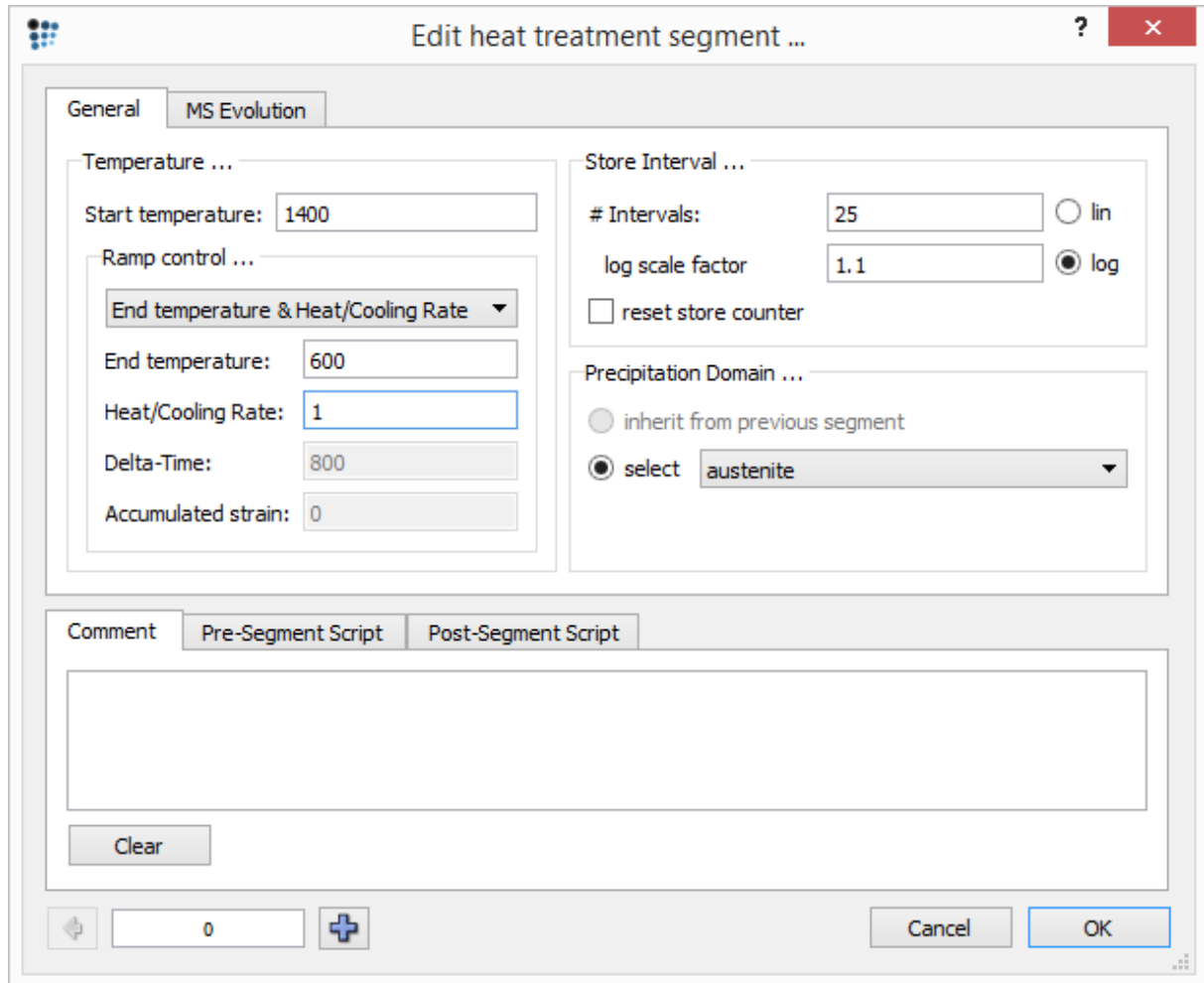


Firstly, create a new treatment by clicking '**New ...**' with the name '**sample_ht**'.

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:



Edit heat treatment segment ...

General | **MS Evolution**

Temperature ...

Start temperature: 1400

Ramp control ...

End temperature & Heat/Cooling Rate ▾

End temperature: 600

Heat/Cooling Rate: 1

Delta-Time: 800

Accumulated strain: 0

Store Interval ...

Intervals: 25 ☐ lin

log scale factor: 1.1 ☒ log

☐ reset store counter

Precipitation Domain ...

☐ inherit from previous segment


☒ select: austenite ▾

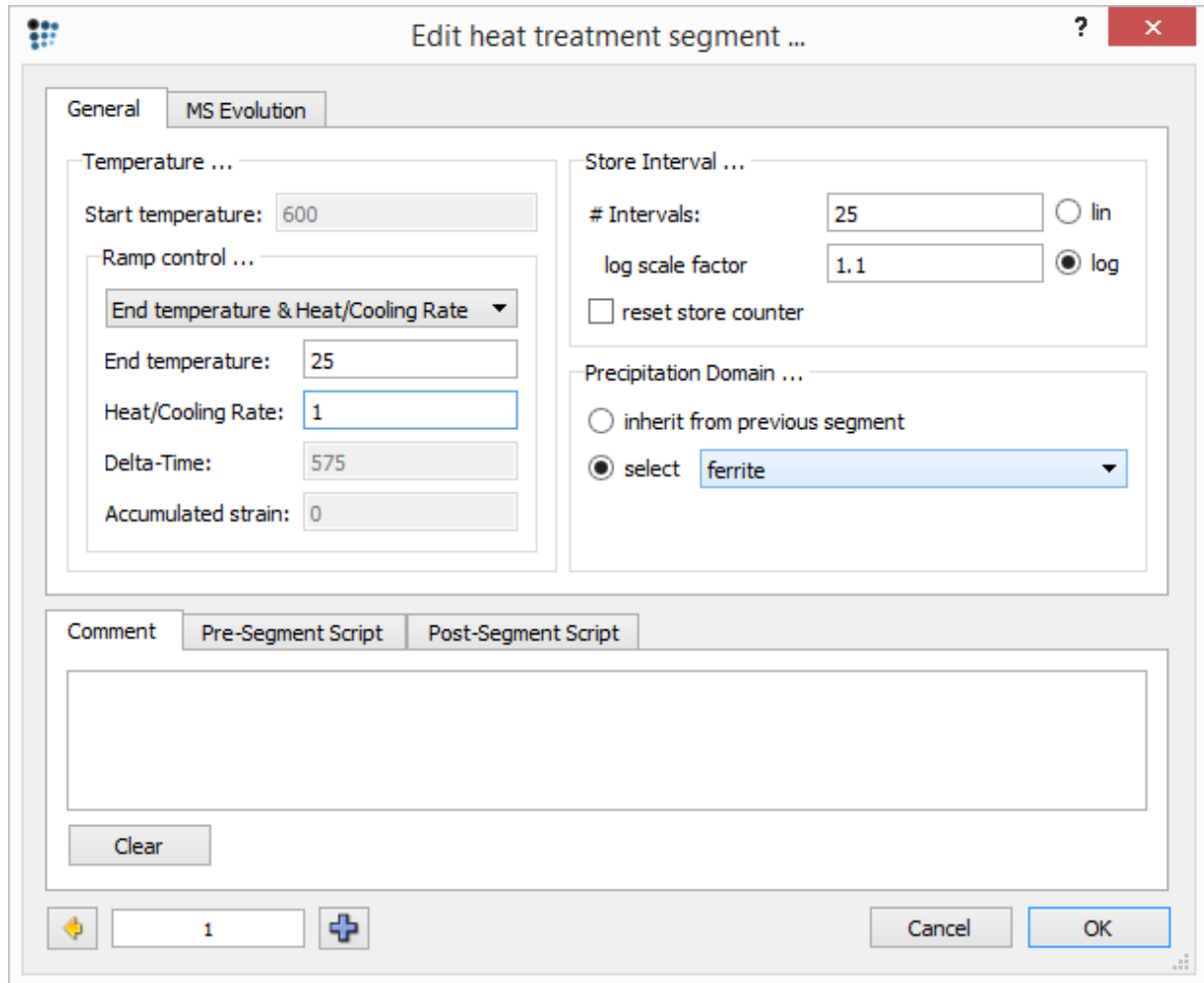
Comment | Pre-Segment Script | Post-Segment Script

Clear

← 0 → +

Cancel OK

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:



Edit heat treatment segment ...

General | **MS Evolution**

Temperature ...

Start temperature: 600

Ramp control ...

End temperature & Heat/Cooling Rate ▾

End temperature: 25

Heat/Cooling Rate: 1

Delta-Time: 575

Accumulated strain: 0

Store Interval ...

Intervals: 25 ☐ lin

log scale factor: 1.1 ☒ log

☐ reset store counter

Precipitation Domain ...

☐ inherit from previous segment

☒ select: ferrite ▾

Comment | **Pre-Segment Script** | **Post-Segment Script**

Clear

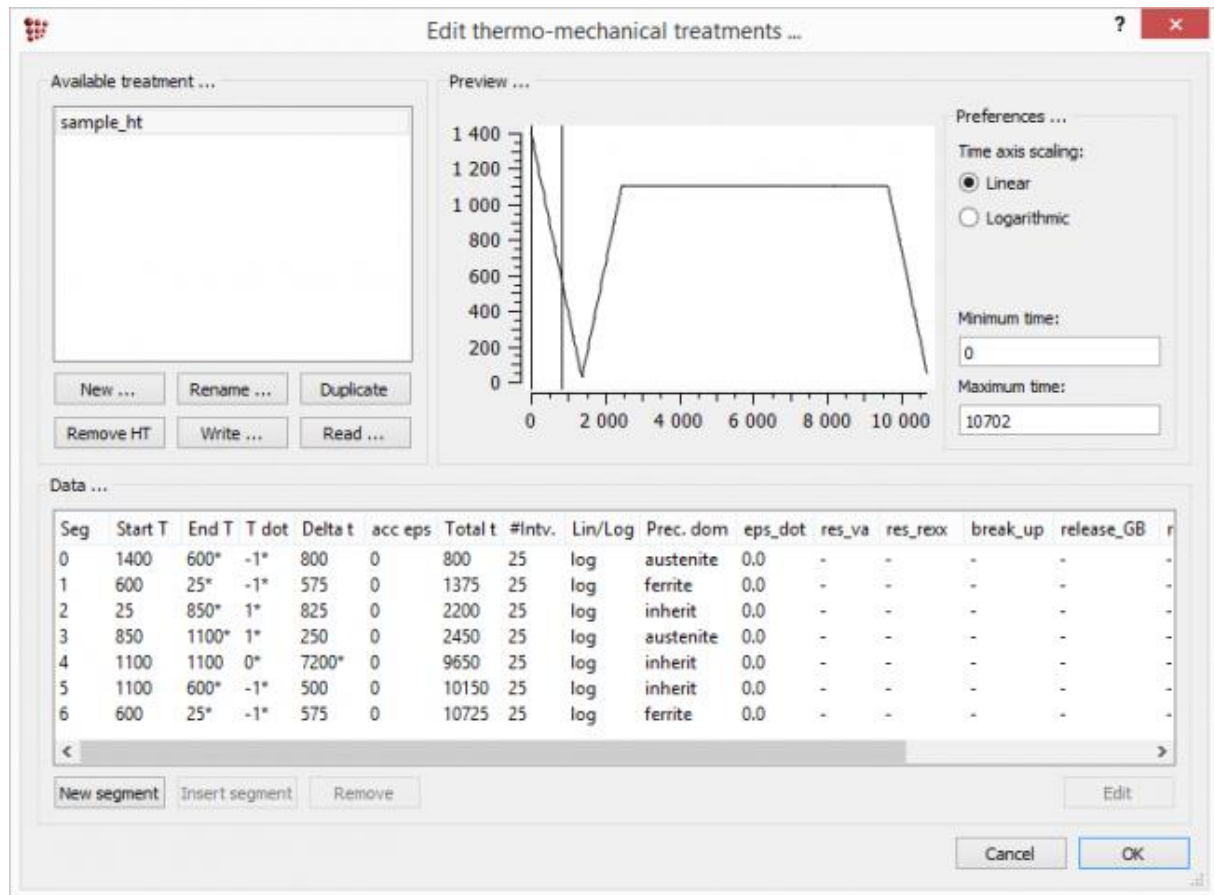
1

Cancel OK

Continue to define the rest of the segments:

1. 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.
2. Next segment from 850°C to 1100°C, however, with austenite as the precipitation domain (heating rate 1 K/s).
3. an isothermal segment for two hours at 1100 °C. This time, the temperature definition mode is '**Heat/Cooling Rate & Delta-Time**'. Heat/Cooling rate 0°C/s and '**Delta-time**' is 7200 s (you can enter 2*60*60 as well).
4. Define a cooling segment down to 600°C in austenite matrix (cooling rate 1 K/s).
5. 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
```

Edit heat treatment segment ...

General **MS Evolution**

Temperature ...
 Start temperature: 1400

Ramp control ...
 End temperature & Heat/Cooling Rate ▾
 End temperature: 600
 Heat/Cooling Rate: -1
 Delta-Time: 800
 Accumulated strain: 0

Store Interval ...
 # Intervals: 25 ☐ lin
 log scale factor: 1.1 ☒ log
☐ reset store counter

Precipitation Domain ...
☐ inherit from previous segment
☒ select austenite ▾

Comment **Pre-Segment Script** **Post-Segment Script**

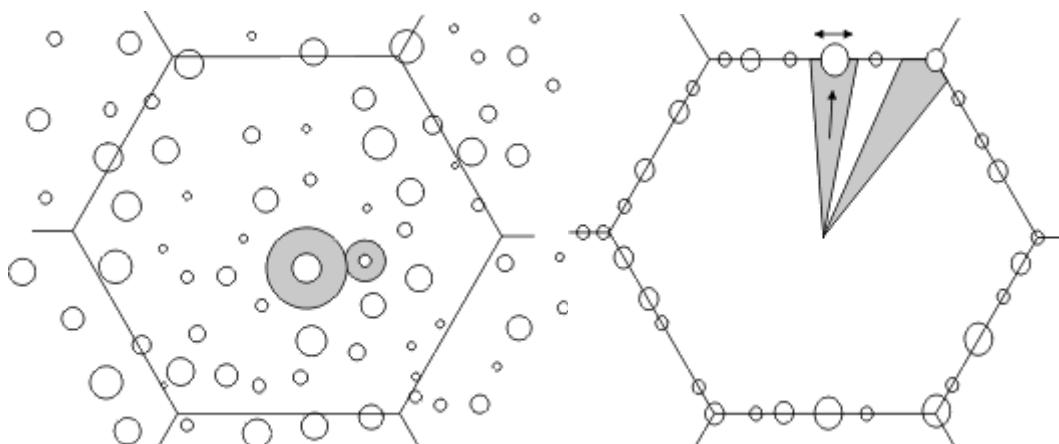
set-precipitation-parameter fcc_a1#01_p0 n s g

Clear

0

Cancel OK

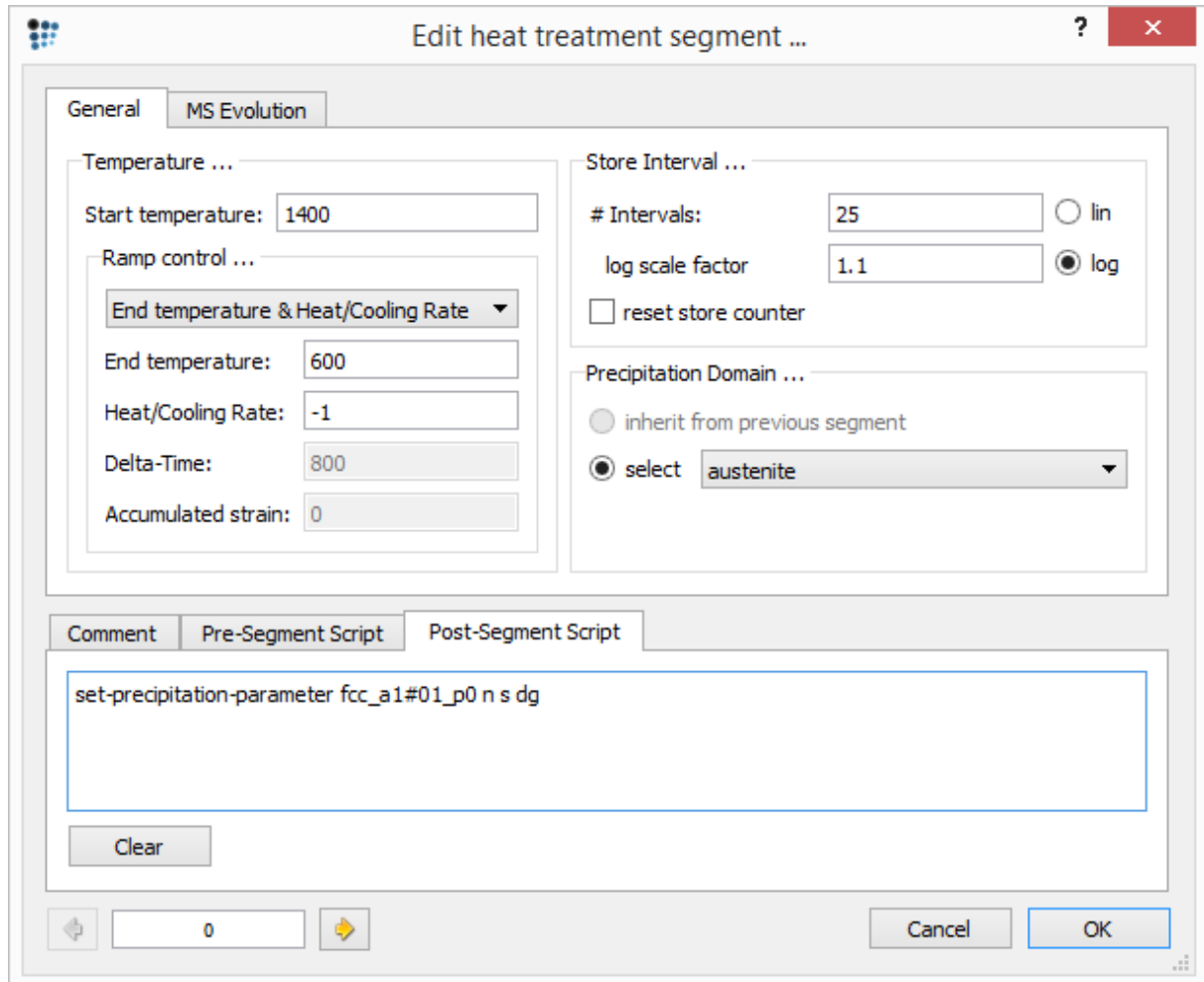
This command defines the (n)ucleation (s)ites of the NbC to be at (g)rain boundaries. Since only grain boundaries are selected, please note that MatCalc will then use the diffusion geometry for grain boundary precipitates, which has been introduced MatCalc version 5.14. The following images show the 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 ('**Tutorial_17.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.

Precipitation kinetics ...

Simulation control ...

Simulation end time:

Simulation end temperature:

Temperature control ...

☐ isothermal: T_iso:
☐ continuous: T_dot:
☒ from heat treatment:

☒ Temperature in C

Maximal T-step:

Composition control ...

element	condition
C	(none)
NB	(none)

Results ...

Buffer:
☐ append to buffer

Update output every:

Store results every ...

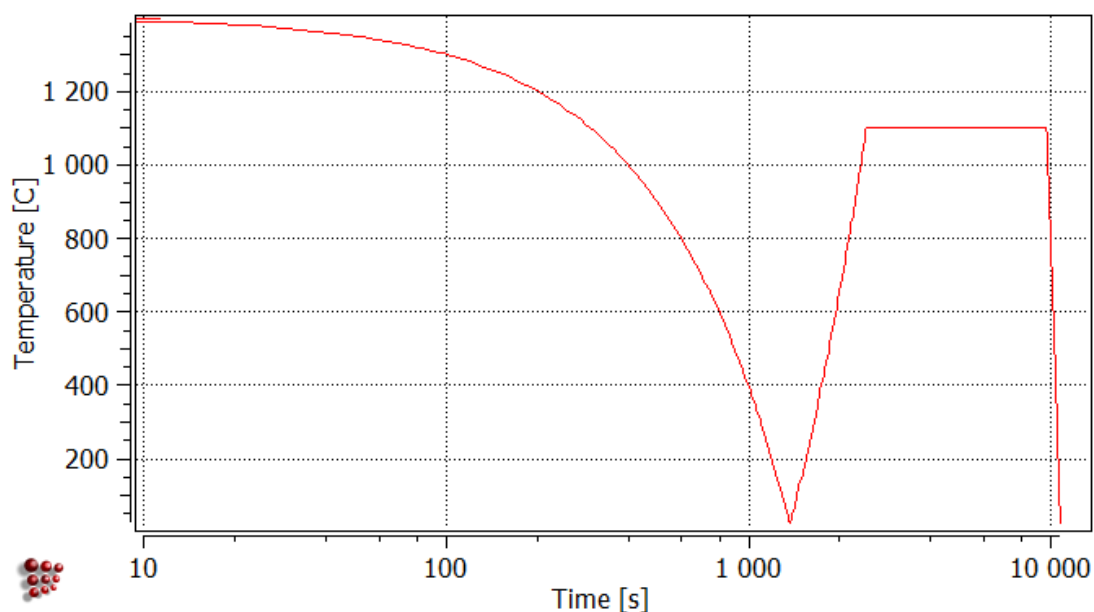
☐ iteration
☐ linear time step width
☒ log time step factor

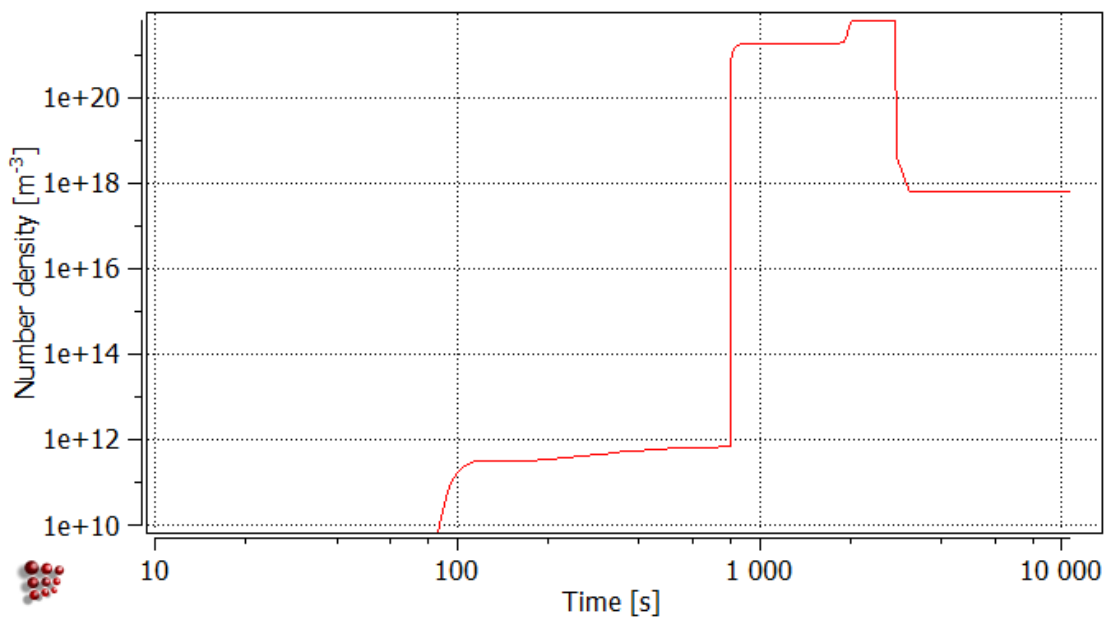
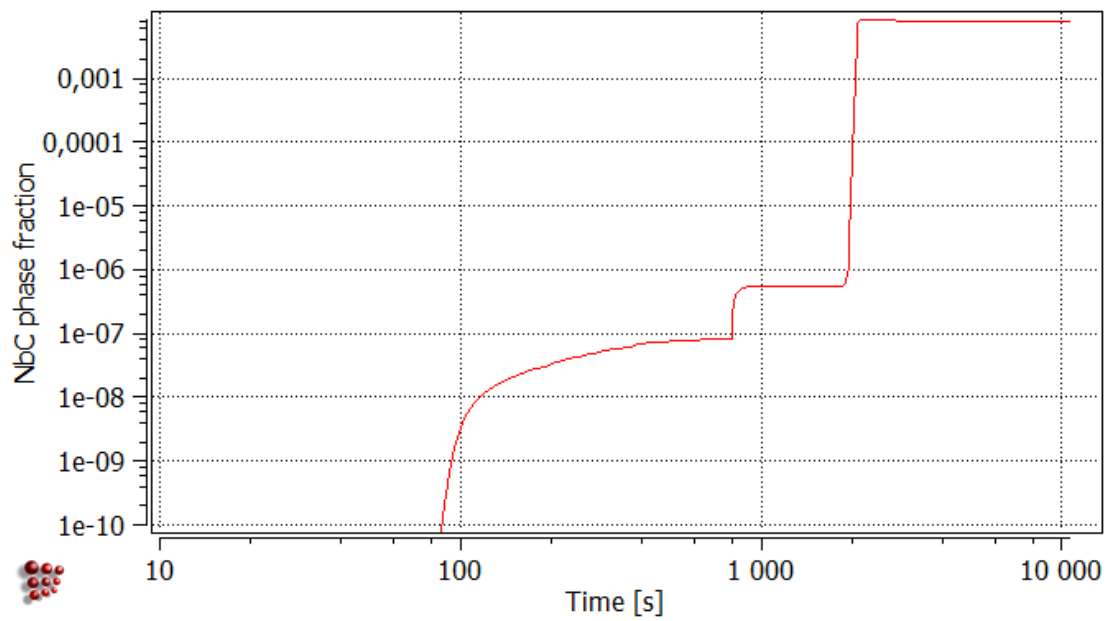
Starting conditions ...

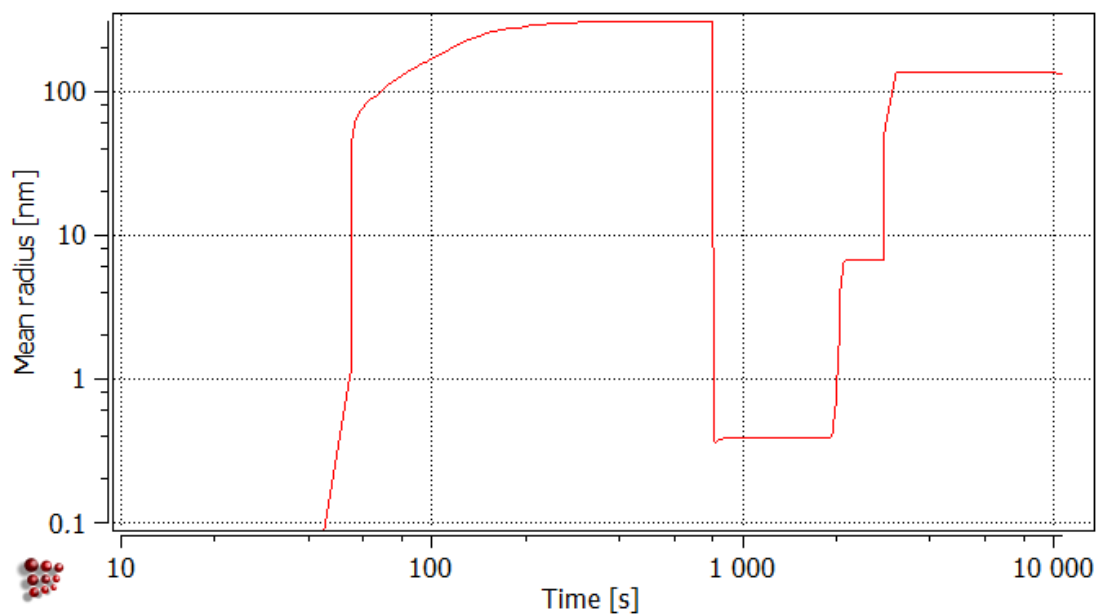
☐ no action
☒ reset precipitates
☐ load from state

Start the precipitation simulation with the 'Go' button.

After reaching the end of the heat treatment, the results look like follows (phase fraction is shown in logarithmic scale):







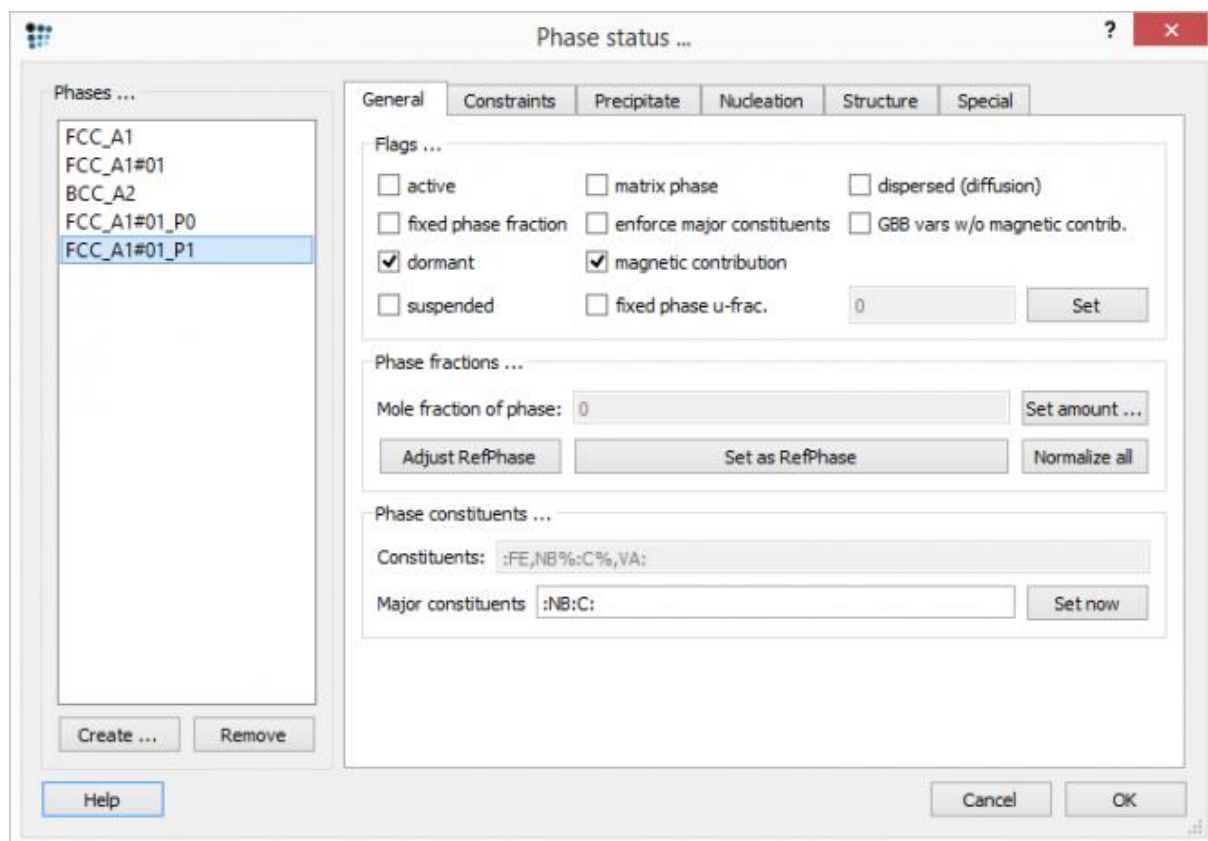
The temperature plot on top shows the expected profile. The next plot with the NbC phase fraction shows a strong increase of the phase fraction at around 80s, where the specimen is at $\sim 1300^{\circ}\text{C}$ on heating. Next, the phase fraction increases when the ferrite region is entered which is due to the lower solubility of NbC in ferrite compared to austenite. The next increase is observed in ferrite domain when the specimen is heated from room temperature. Later, during austenitization, the phase fraction is decreased slightly (better seen with the linear scale for phase fraction) 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 ~ 100 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.



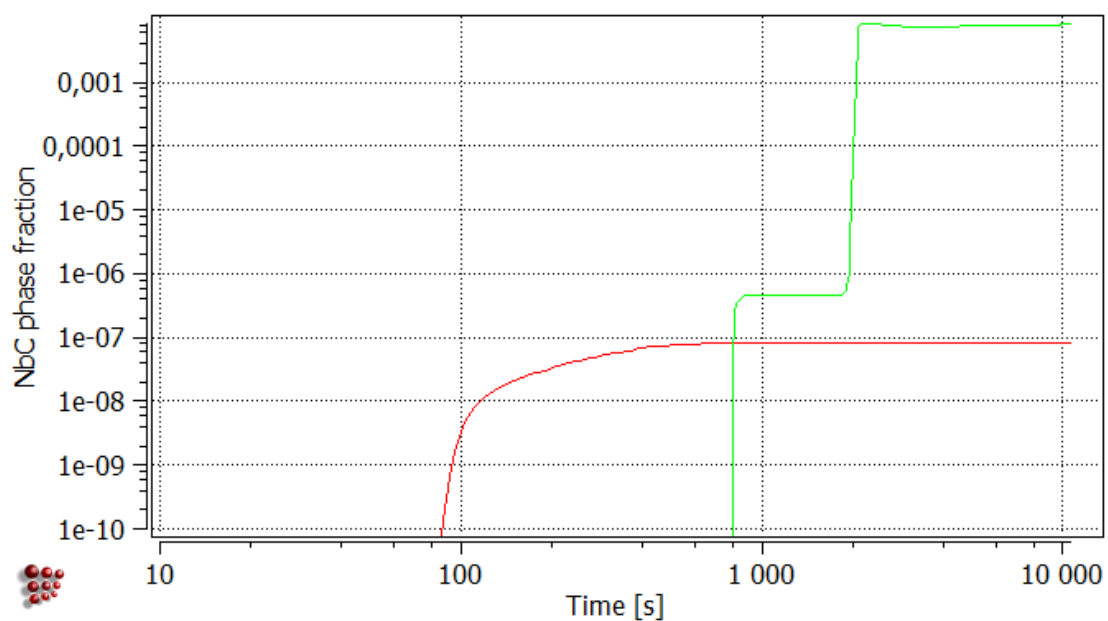
Note that the suffix '**_P1**' of the new phase indicates that the precipitate is identical to the '**_P0**' in terms of its nucleus composition, however, it contains precipitate classes that can have appeared at different stages of the heat treatment.

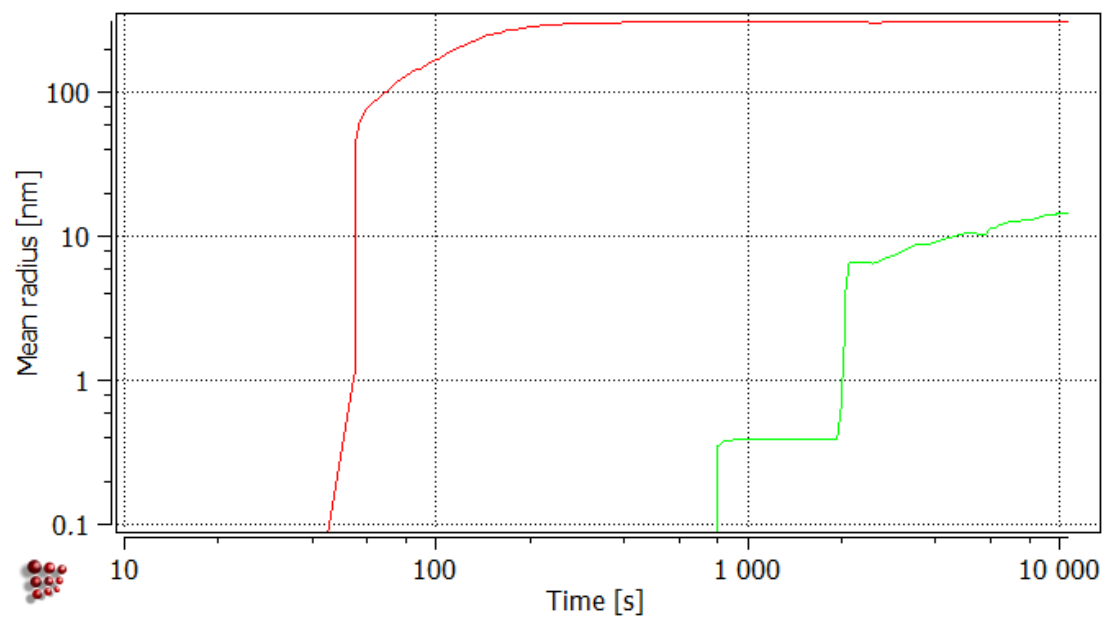
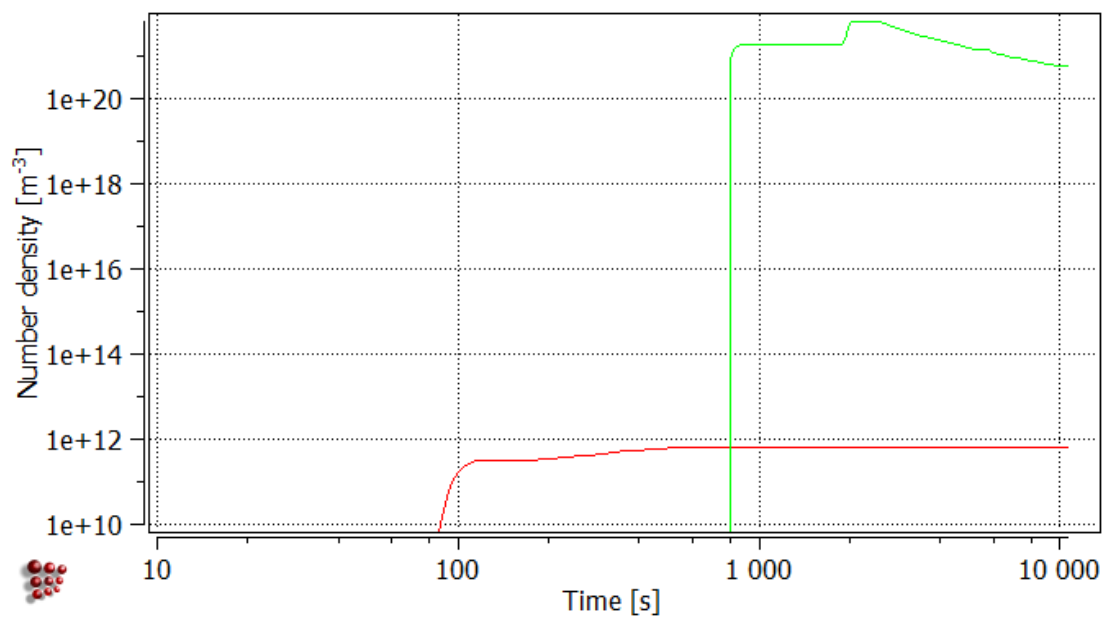
Let us now set up the simulation such that the _P0 phase can only nucleate in the first segment of the heat treatment, that is cooling in the austenite, while the '**_P1**' population is not allowed to form. This can be done by defining '**nucleation sites**' as '**none**'. For all consecutive segments,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

Comment	Pre-Segment Script	Post-Segment Script
	<pre>set-precipitation-parameter fcc_a1#01_p0 n s g set-precipitation-parameter fcc_a1#01_p1 n s n</pre>	
	<input type="button" value="Clear"/>	

Comment	Pre-Segment Script	Post-Segment Script
	<pre>set-precipitation-parameter fcc_a1#01_p0 n s n set-precipitation-parameter fcc_a1#01_p1 n s dg</pre>	
	<input type="button" value="Clear"/>	

Run the simulation again and modify the plots (add the series relevant for the FCC_A1#01_P1 phase) to display the properties of both precipitate populations. The result should look like this:



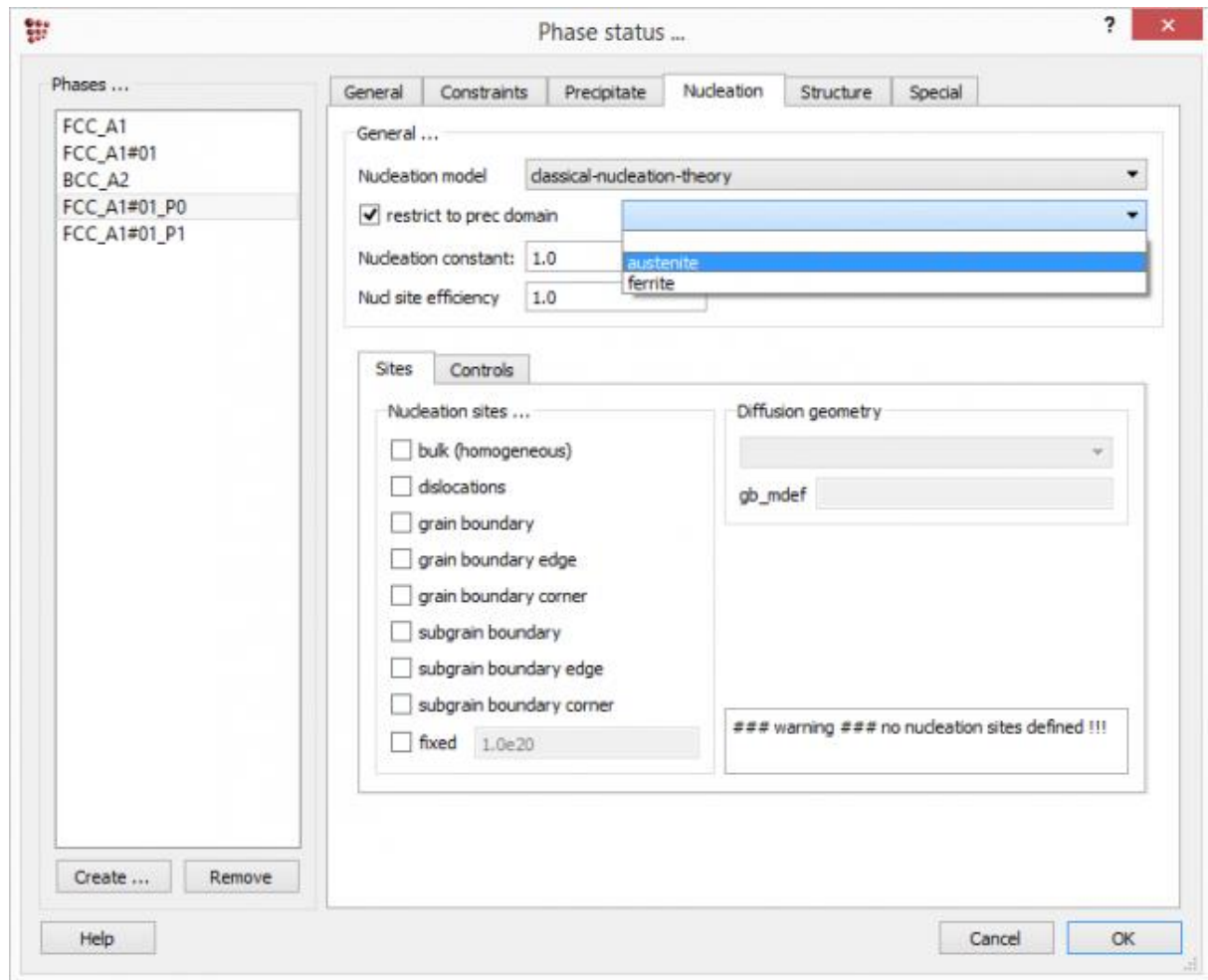


Major advantage of simulations with separated precipitate populations is the ease of interpretation of the results. The second simulation clearly shows that the precipitates that are formed during cooling in the austenite grow to large size and remain almost unaltered during the later stages of the heat 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 material strengthening of this second wave of NbC precipitates.

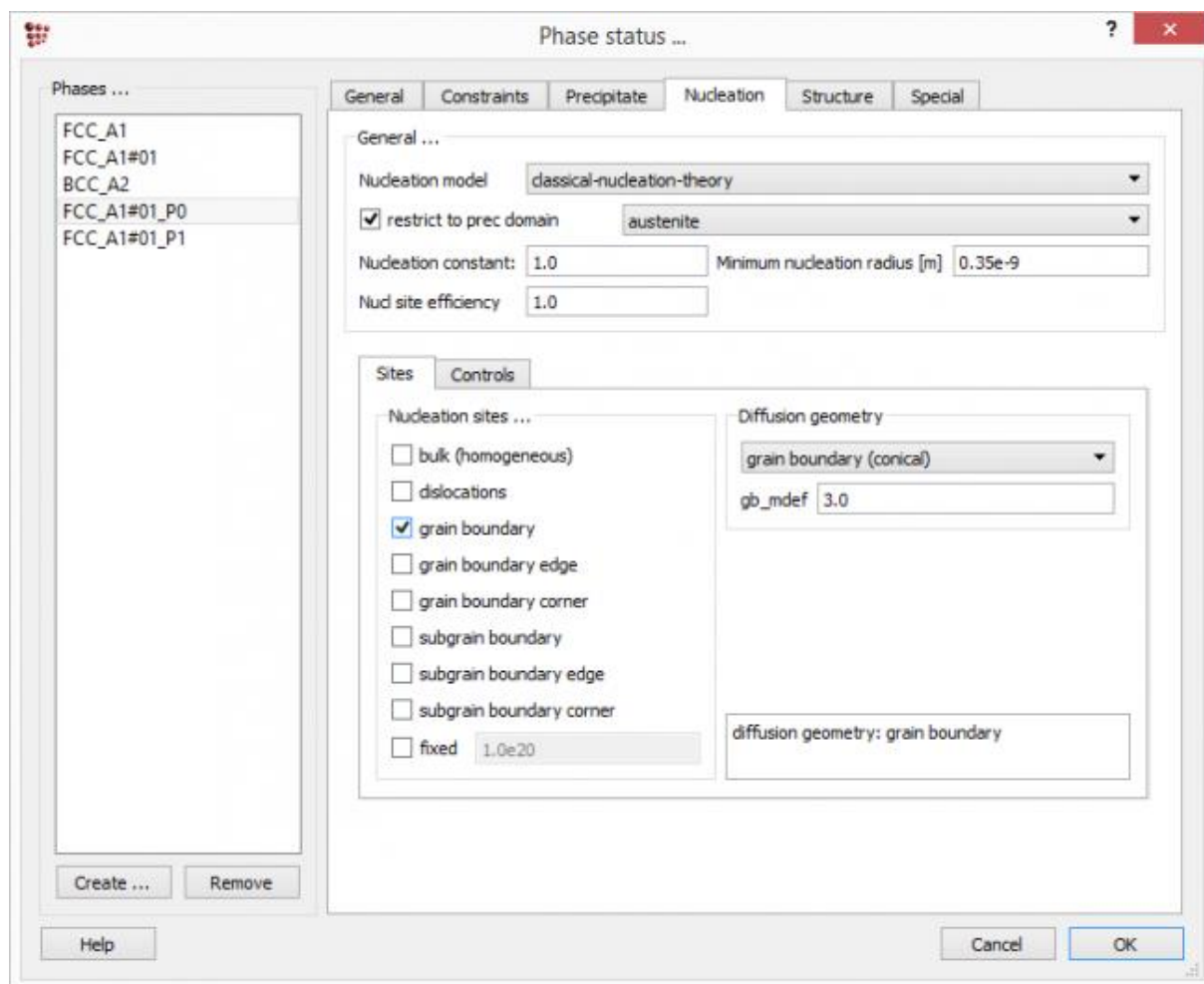
RESTRICTING PRECIPITATE NUCLEATION TO THE SELECTED PRECIPITATE DOMAIN

The difference between the FCC_A1#01_P0 and FCC_A1#01_P1 precipitate phases lies in their nucleation sites. FCC_A1#01_P0 represents the precipitate formed on the austenite grain boundaries during the continuous cooling, while FCC_A1#01_P1 represents the precipitate formed mainly in the ferrite region on both the dislocations and the grain boundaries. As the switch between the two precipitate phases coincides with the switch of the precipitation domains, an alternative implementation of the two phases population is possible, where each precipitate phase is restricted to form in the selected precipitation domain only.

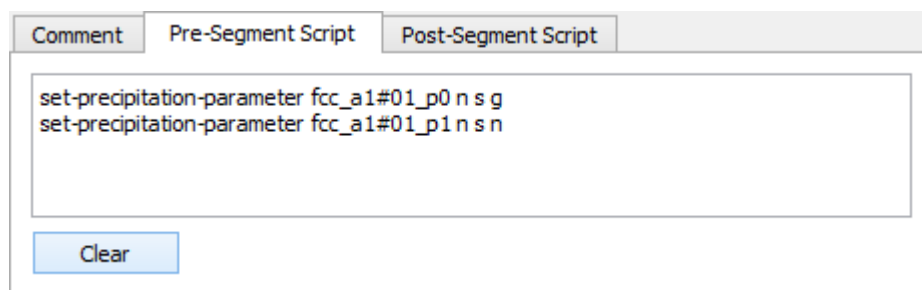
Go to '**Global**' > '**Phase status**' and select '**FCC_A1#01_P0**' phase. In the '**Nucleation**' tab mark the '**restrict nucleation to prec domain**' field and select '**austenite**' in the adjacent drop-box.



Repeat this for the '**FCC_A1#01_P1**' phase, but select '**ferrite**' as the precipitation domain. Next, have a look on the nucleation sites of those phases. The content of the tab represents the final state of the last simulation. Hence, the dislocations and the grain boundaries are selected for the '_P1'-phase, but no nucleation sites are selected for the '_P0'-phase. Again, select '**grain boundary**' as nucleation sites for the '**FCC_A1#01_P0**' phase.



With these settings, the pre- and post-scripts are not needed anymore. To remove those, go to the **'Global' > 'Heat treatments'** and click on the very first segment in the **'Data...'** list box. In the segment editor dialog, click on the **'Clear'** button below the content of the post-segment script. Select the **'Pre-Segment Script'** tab and click on the **'Clear'** button again. Close the heat treatment editor.



Duplicate and lock all series and start the simulation. The results look virtually identical with the previous simulation.

T18: PLOTTING A TTP DIAGRAM

This tutorial was tested on

MatCalc version 6.00 rel 0.100

license: free

database: mc_fe.tdb; ; mc_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.

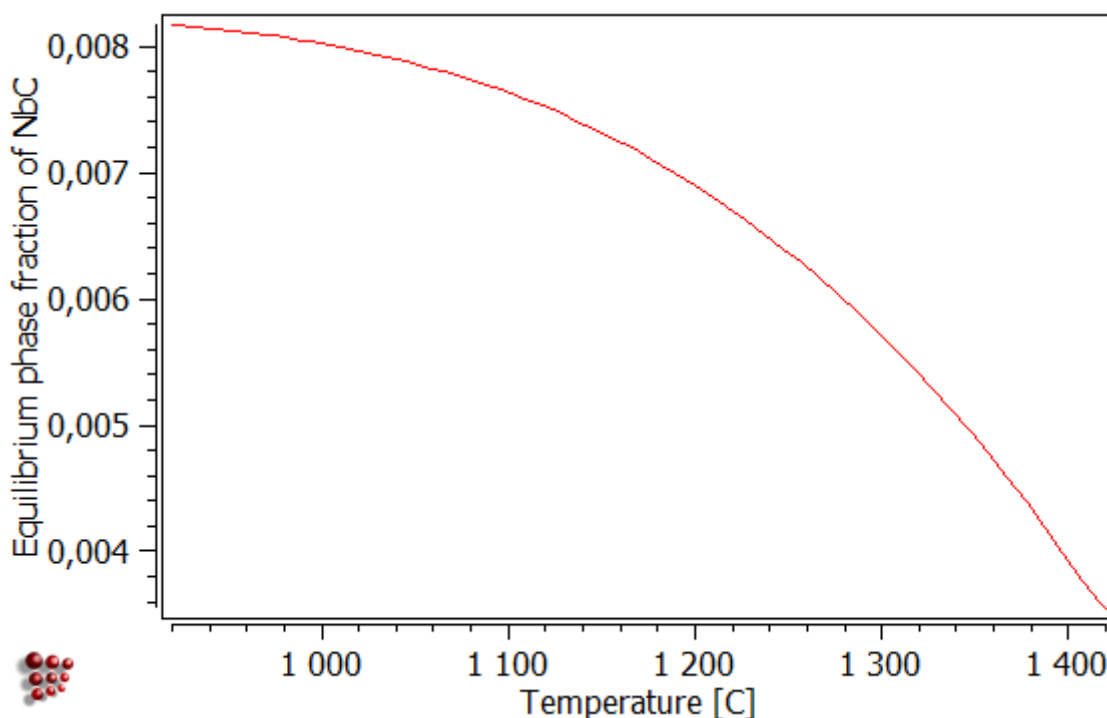
SETTING UP THE SYSTEM

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 905.24°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 1397.68°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 900°C and 1400°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. Its precipitation sites should be dislocations. Leave all the other settings at their default values. Read in the mobility data.

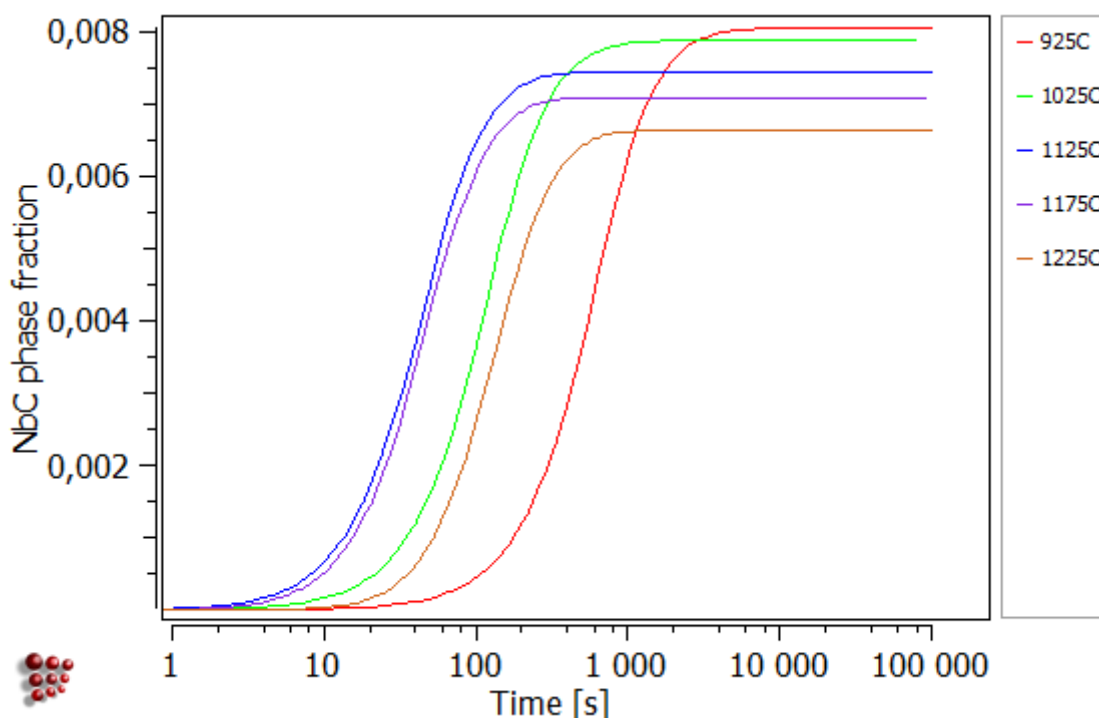
TTP DIAGRAMS FOR ISOTHERMAL HEAT TREATMENTS

CALCULATIONS OF PHASE FRACTION FOR ISOTHERMAL TREATMENTS

The plot below, obtained using a stepped equilibrium calculation, shows the equilibrium phase fraction of NbC between 900 and 1400°C:



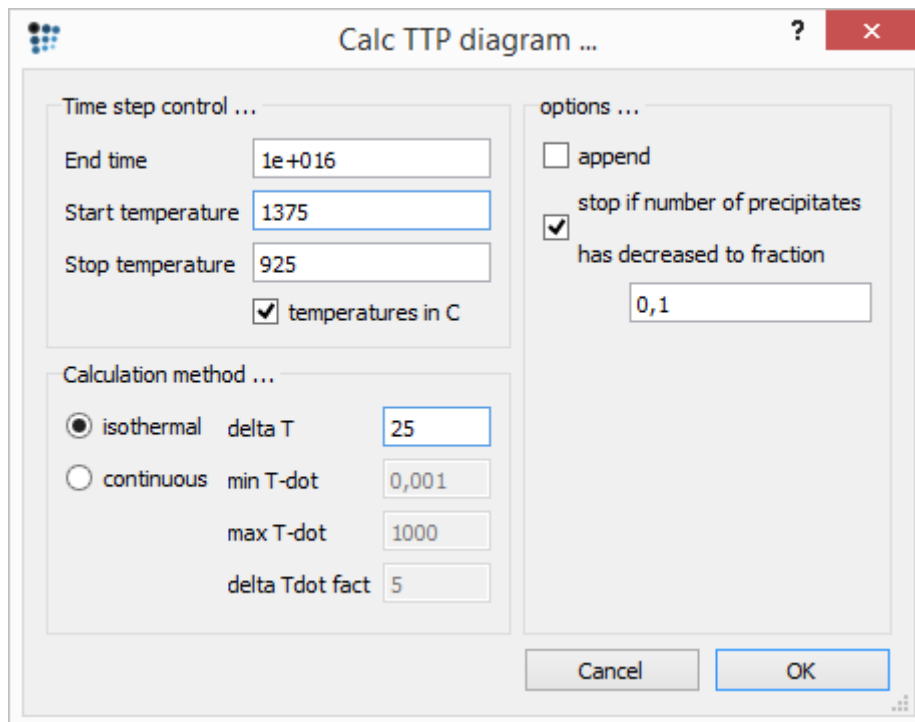
The plot below illustrates the origin of the typical C-shaped curves of TTP plots. It was obtained using '**Calc > Precipitation kinetics**' to simulate an isothermal heat treatment at 925°C, plotting the series **F\$FCC_A1#01_P0** on a logarithmic x-axis, then duplicating and locking this series before 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 1100 and 1200°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 '**1375**' 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

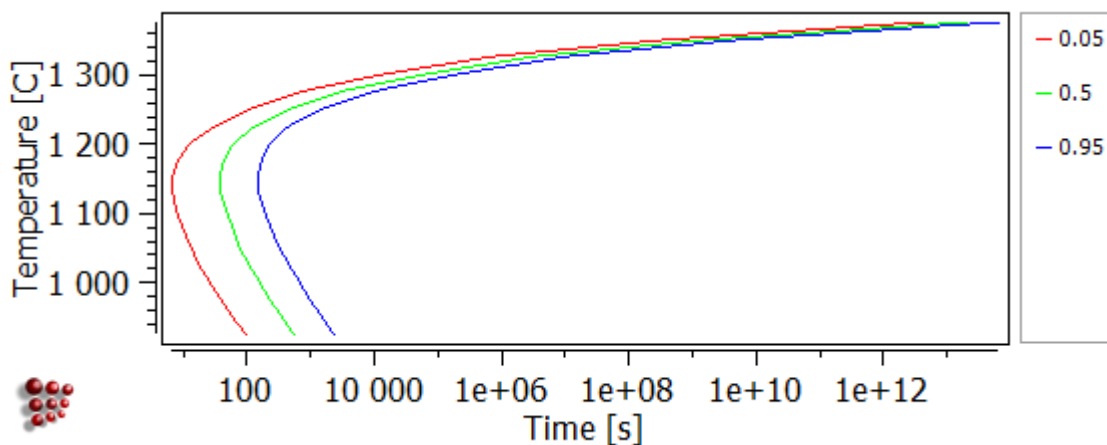
When the calculation has finished, create a new window of type '**(p6) Plot: TTP-diagram**'. In the '**options**' window, expand the '**plots**' section and right-click in the area under '**plot#0**' to show the context menu. Select '**new series**' and choose '**ttp-curve**' from the sub-menu on the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

option	value
series	
series #0	
name	auto
type	ttp-curve
locked	yes
deriva...	0
conne...	
x-data	---
y-data	0,05
phase	FCC_A1#01_P0
default...	yes
line	
marker	

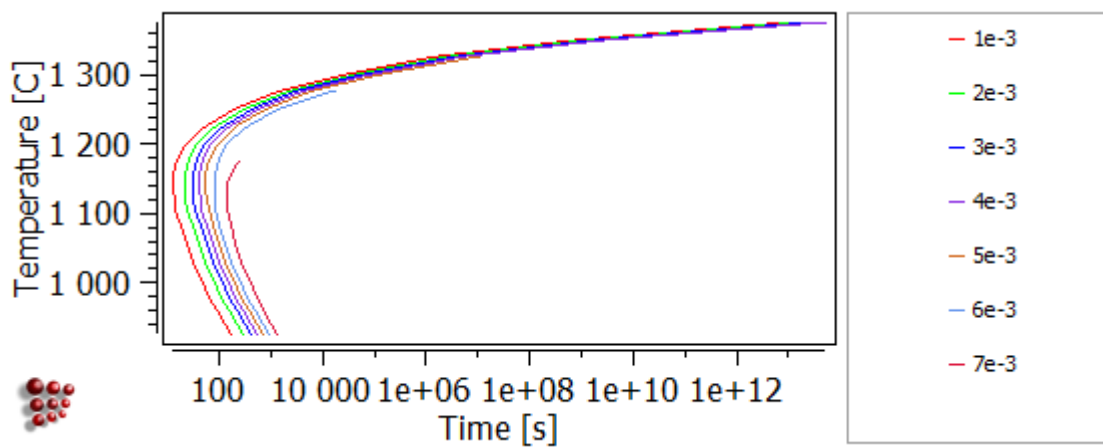
Add two more series to show the contours for ratios of 0.5 and 0.95 on the same diagram. The resulting diagram should look like this:



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.)

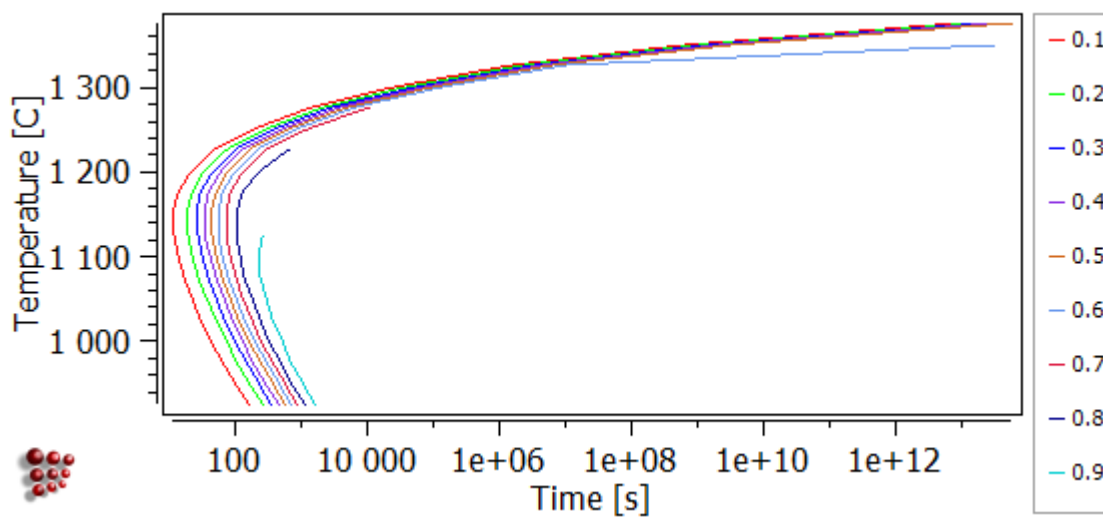
ABSOLUTE

In the plot below, the contours correspond to different values of the phase fraction $F_{\text{FCC_A1\#01_P0}}$. Note that the higher values are only attained at lower temperatures, because the equilibrium value of $F_{\text{FCC_A1\#01}}$ decreases with increasing temperature. The maximum value of $F_{\text{FCC_A1\#01_P0}}$ is around 7.8×10^{-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.



T19: SCRIPTING PRECIPITATION CALCULATIONS

This tutorial was tested on

MatCalc version 6.00 rel 0.051

license: free

database: mc_fe.tdb, mc_fe.ddb

The use of **scripting** to help ensure repeatability of calculations and to simplify repetitive operations has been introduced for the equilibrium calculations [Tutorial 13](#). The present tutorial describes how scripting can be used for precipitation calculations.

CONTENTS

- Setting up precipitation domains
- Setting up precipitate phases
- Scripting a complex heat-treatment
- Modifying precipitation parameters during heat-treatment
- Plotting using scripts

The example used here uses the already familiar Fe-Nb-C system and considers a heat-treatment of an initially well-annealed ferritic microstructure with no primary precipitates. Cementite is initially allowed to nucleate on dislocations, and NbC on grain boundaries. The microstructure is heated into the austenite phase stability region, held isothermally and then cooled quickly (quenched). On quenching, a martensitic transformation occurs. This is modelled in MatCalc by a modification of the ferrite precipitation domain to increase the dislocation density as well as the addition of subgrains as possible nucleation sites for the NbC phase. The system is then subjected to a tempering heat treatment consisting of heating, isothermal hold and cooling stages.

SETTING UP THE SYSTEM AND THERMODYNAMICS

Start the script by with two lines to make sure the right module (the core module) is used, and to create a new workspace:

```
use-module core

new-workspace $ creates a new workspace
```

The following code can be used to check that the correct version of MatCalc is being used. This is useful when scripts rely on functionality that is only available in newer versions of the software. The code `send-dialog-string` sends a message to the user in the form of a dialogue box, and `stop-run-script` prevents any further commands from being executed.

```
if (matcalc_version<6000000)

    send-dialog-string "MatCalc version must be 6.00.0000 or higher to run this
script. Stopping."

    stop-run-script

endif
```

Scripts should be well commented to ensure that they can be easily understood later. See Tutorial 13 for a reminder of how comments are inserted.

Some information on the physical situation to be modelled and the assumptions made can be inserted into the MatCalc workspace for future reference.

```
@$*****

$ enter workspace info

@$*****

@ set-workspace-info Script T19

@ set-workspace-info +Calculation of precipitation

@ set-workspace-info +in Fe-0.1C-0,7Nb wt.% system

@ set-workspace-info +during a complex heat treatment

@ set-workspace-info +with phases BCC_A2, FCC_A1 and CEMENTITE.
```

The thermodynamic setup is then carried out. Firstly, the database is chosen and the elements and phases are selected. The database is then read.

```
open-thermodyn-database mc_fe.tdb
```

```
select-elements FE C NB VA  
select-phases BCC_A2 FCC_A1 CEMENTITE  
read-thermodyn-database
```

The composition is entered:

```
set-reference-element FE  
enter-composition WP C=0.1 NB=0.7
```

and an equilibrium is calculated, after setting automatic start values.

```
set-temperature-celsius 1000  
set-automatic-startvalues  
calculate-equilibrium
```

SETTING UP THE PRECIPITATION DOMAINS

We proceed by creating the precipitation domains. The calculation involves heat-treatment in both ferrite (BCC_A2) and austenite (FCC_A1) phase stability regions, so we start by creating these two domains.

```
create-precipitation-domain ferrite  
create-precipitation-domain austenite
```

We must then tell MatCalc with which matrix phases to associate these domains:

```
set-precipitation-parameter ferrite X BCC_A2  
set-precipitation-parameter austenite X FCC_A1
```

Structural parameters are then defined for ferrite (note comments describing the meanings of the commands):

```
$ In S[t]ructure, [e]quilibrium) [d]islocation density set to 1e12  
set-precipitation-parameter ferrite T D E 1e12  
$ In S[t]ructure, [g]rain diameter set to 100e-6  
set-precipitation-parameter ferrite T G 100e-6  
$ In S[t]ructure, [s]ubgrain diameter is set to 10e-6  
set-precipitation-parameter ferrite T S 10e-6
```



```
$ In S[t]ructure, subgrain el[ongation factor set to 10  
set-precipitation-parameter ferrite T O 10
```

and for austenite. Note that for ferrite, parameters characterising the subgrains are included because subgrain boundaries will be used as nucleation sites later in the calculation. In austenite, this is not the case so the parameters for this domain are not relevant and need not be set.

```
$ In S[t]ructure, [e]quilibrium)[d]islocation density set to 1e12  
set-precipitation-parameter austenite T D E 1e12  
$ In S[t]ructure, [g]rain size section, the grain diameter is set to 100e-6  
set-precipitation-parameter austenite T G 100e-6
```

SETTING UP THE PRECIPITATE PHASES

The next stage in the script is to set up the precipitates. Firstly, we need to create precipitate phases from the equilibrium phases.

```
create-new-phase CEMENTITE P  
create-new-phase FCC_A1#01 P
```

Note that this latter phase is derived from the second FCC_A1 phase, FCC_A1#01, which is automatically generated by MatCalc, based on a command in the database, as a result of the presence of the MX carbonitride former, Nb, in the system.

The precipitate phase are initialised with 100 size classes each.

```
set-precipitation-parameter CEMENTITE_P0 C 100  
set-precipitation-parameter FCC_A1#01_P0 C 100
```

Then the nucleation sites are defined:

```
$ In the [n]ucleation section, the nucleation [s]ites are set to [d]islocations  
set-precipitation-parameter CEMENTITE_P0 N S D  
$ [G]rain boundaries are [n]ucleation [s]ites for NbC precipitate  
set-precipitation-parameter FCC_A1#01_P0 N S G
```

The nucleus composition of the iron-rich cementite precipitate phase is set to para-equilibrium, and that of NbC is set to ortho-equilibrium.

```
$ In the [n]ucleation section, the nucleus [c]omposition is set to [p]ara-  
composition  
  
set-precipitation-parameter CEMENTITE_PO N C P  
  
$ [O]rtho-[c]omposition for the NbC precipitate [n]uclei  
  
set-precipitation-parameter FCC_A1#01_PO N C O
```

Finally, the mobility database is read in:

```
read-mobility-database mc_fe.ddb
```

HEAT-TREATMENT

For an isothermal precipitation simulation, we would now simply need to set the temperature and time and start the simulation. This procedure is described briefly [below](#). However, we will here instead look at how to use a script to create a heat-treatment.

The heat-treatment consists of two sections:

An austenitisation and quenching treatment consisting of:

- heating from room temperature to the austenitisation temperature; since this heating step involves a phase transformation from ferrite to austenite, this must be specified in two stages - heating up to the transformation temperature with a ferrite precipitation domain, and then heating from the transformation temperature with an austenite precipitation domain.
- an isothermal hold at the austenitisation temperature

quenching to room temperature; again, this is separated into two stages, the first of which has an austenite precipitation domain, and the second, a ferrite precipitation domain.

- A tempering treatment consisting of:
 - heating from room temperature to the tempering temperature
 - an isothermal hold at the tempering temperature
 - cooling to room temperature

The tempering treatment is carried out entirely in the ferrite phase stability region, so no change of precipitation domain is necessary.

Start by creating a heat treatment sequence called `sample_ht`.

```
create-heat-treatment sample_ht
```

Heat- or thermomechanical treatments can consist of different types of segments. In this tutorial, we will use two of these:

- **Type 1:** this consists of an end temperature and a heating/cooling rate (use a negative sign to specify cooling)
- **Type 3:** this consists of an end temperature and a time.

We saw in Tutorial 6 that it is possible to define our own variables. Here, we use this functionality to define a very general script consisting of an austenitisation and a tempering step.

```
set-variable-value f_a_temp 850 $ferrite-> austenite transformation temp. in C
set-variable-value a_f_temp 600 $austenite-> ferrite transformation temp. in C
set-variable-value aus_temp 1100 $austenitisation temp. in C
set-variable-value temp_temp 600 $tempering temp. in C
set-variable-value rate_heat_to_aus 1 $rate of heating to aus_temp in K/s
set-variable-value rate_cool_from_aus -10 $rate of cooling from aus_temp in K/s
set-variable-value rate_heat_to_temp 1 $rate of heating to temp_temp in K/s
set-variable-value rate_cool_from_temp -1 $rate of cooling from temp_temp in K/s
set-variable-value aus_time 3600 $austenitisation time in seconds
set-variable-value temp_time 7200 $tempering time in seconds
```

AUSTENITISATION AND QUENCHING TREATMENT

Start by adding the **first segment**, using the command

```
append-ht-segment sample_ht
```

Then specify the [s]tart temperature. The notation `[.]` means **the current segment**. It is also possible to refer to the segments by number.

```
edit-ht-segment sample_ht . S 20
```

This first segment consists of heating, at a rate **rate_heat_to_aus** up to the temperature **f_a_temp** at which the ferrite-austenite phase transformation takes place.

The parameters for the segment are thus set; the parameter set no.[1] is chosen with end temperature **f_a_temp** and heating rate **rate_heat_to_aus** K/s.

```
edit-ht-segment sample_ht . 1 f_a_temp rate_heat_to_aus
```

The precipitation [d]omain associated with this segment must now be set, as it is [n]ot inherited from any previous

```
edit-ht-segment sample_ht . D N ferrite
```

We then append a **new segment** to accommodate the remainder of the heating ramp to the austenitisation temperature.

```
append-ht-segment sample_ht
```

This new segment now becomes the current segment, so we can modify *its* parameters using the [.] notation. Again, the parameter set [1] is chosen with end temperature **aus_temp** and the same heating rate, **rate_heat_to_aus**, as before.

```
edit-ht-segment sample_ht . 1 aus_temp rate_heat_to_aus
```

We also need to change the precipitation [d]omain, so that it is [n]ot inherited from the previous segment but is instead set to austenite:

```
edit-ht-segment sample_ht . D N austenite
```

The next stage is the isothermal hold. Add a **new segment**.

```
append-ht-segment sample_ht
```

The isothermal hold is specified using parameter set type [3], with end temperature **aus_temp** and hold time **aus_time**.

```
edit-ht-segment sample_ht . 3 aus_temp aus_time
```

The precipitation domain (austenite) is inherited from the previous segment.

```
edit-ht-segment sample_ht . D Y
```

We next add two segments for cooling down from the austenitisation domain to room temperature. Add a **new segment** for the austenite domain part. Set the segment type to [1] and set the end temperature to the austenite-ferrite transformation temperature **a_f_temp** and the cooling rate to **rate_cool_from_aus**. Set the segment to **inherit** the precipitation domain (austenite).

```
append-ht-segment sample_ht  
edit-ht-segment sample_ht . 1 a_f_temp rate_cool_from_aus  
edit-ht-segment sample_ht . D Y
```

Add a further **new segment** for the ferrite domain part. In this case, we again use type [1] and, this time, set the end temperature to 20 and the cooling rate, as before, to **rate_cool_from_aus**. This time, the precipitation domain is not inherited, but is instead set to **ferrite**.

```
append-ht-segment sample_ht  
edit-ht-segment sample_ht . 1 20 rate_cool_from_aus  
edit-ht-segment sample_ht . D N ferrite
```

In addition, since this ferrite is now quenched martensite, we make some modifications to the properties of the precipitation domain. As we saw in [Tutorial 17](#), pre- and post-segment scripts can be appended to segments of a thermomechanical treatment. The syntax for these scripts is illustrated by the following line of code, which sets the equilibrium dislocation density in the ferrite domain to 1e14:

```
edit-ht-segment sample_ht . O +set-precipitation-parameter ferrite T D E 1e14
```

The O here indicates a p[o]st-segment script; a p[r]e-segment script is instead indicated by the letter R in place of the O. The +sign means that the following piece of script is added to any existing commands. An existing command can be removed by prepending a --sign.

Similarly, in the following line, the [n]ucleation [s]ites of FCC_A1#01_P0 are set to include [s]ubgrains as well as [g]rains.

```
edit-ht-segment sample_ht . O +set-precipitation-parameter FCC_A1#01_P0 N S GS
```

TEMPERING TREATMENT

The structure of the tempering treatment is similar to that of the austenitisation treatment, but somewhat simpler, since no phase transformation needs to be considered.

The first part of this treatment is a heating segment with an end temperature of `temp_temp` and a heating rate of `rate_heat_to_temp`. The precipitation domain is inherited from the previous segment.

```
append-ht-segment sample_ht  
edit-ht-segment sample_ht . 1 temp_temp rate_heat_to_temp  
edit-ht-segment sample_ht . D Y
```

This is followed by an isothermal hold for `temp_time` at the tempering temperature `temp_temp`; the precipitation domain is inherited:

```
append-ht-segment sample_ht  
edit-ht-segment sample_ht . 3 temp_temp temp_time  
edit-ht-segment sample_ht . D Y
```

Finally, a cooling segment returns the system to room temperature with a rate of `rate_cool_from_temp`. The precipitation domain is once more inherited.

```
append-ht-segment sample_ht  
edit-ht-segment sample_ht . 1 20 rate_cool_from_temp  
edit-ht-segment sample_ht . D Y
```

PLOTS

The final part of the setup before the calculation is run consists of setting up the plots. We will create four X-Y plots in a single plot window as well as a histogram of precipitate size distribution for each of the precipitate phases.

Start by creating a GUI window of type **p1** (X-Y plot)

```
new-gui-window p1
```

Then set up the default x-axis so that it is used for all the plots in this windows, and has the properties specified below:

```

set-gui-window-property . S U Y                $ Use default x-axis
set-gui-window-property . S T Time [h]          $ Default x-axis title
set-gui-window-property . S Y lin              $ Linear scale
set-gui-window-property . S S 1e-10..          $ Scaling limit x-axis
set-gui-window-property . S F 1/3600           $ Multiplication factor s -> h

```

The first plot will contain the temperature profile as determined by the heat-treatment. The y-axis is labelled accordingly.

```

set-plot-option . S N B T$C %s                $ Temperature in Celsius
set-plot-option . A Y 1 T Temperature [°C]      $ y-axis title

```

The legend box is removed because it is not necessary when only one series is plotted:

```
set-plot-option . L N
```

A new plot is then created in the existing plot window [.] using the command:

```
create-new-plot X .
```

This is set up to show the phase fractions of the two precipitate phases. The syntax %s here means that the MatCalc variables are used as-is without any modification. (See Tutorial 5)

```

set-plot-option . A Y 1 T Phase fraction        $ y-axis title
$ New series: fraction of cementite precipitate phase
set-plot-option . S N B F$CEMENTITE_P0 %s
$ New series: fraction of NbC precipitate phase
set-plot-option . S N B F$FCC_A1#01_P0 %s

```

There are two series in this plot, so we label them. The two series here are referred to by number. The ordering number corresponds to the order in which they appear **in the plot**, not in the plot window, and begins at 0.

```

set-plot-option . S M 0 Cementite      $ Rename series -> "Cementite"
set-plot-option . S M 1 NbC           $ Rename series -> "NbC"

```

A further new plot is created, to plot the number density of precipitates. The series are renamed; note that the numbering starts at 0 again because we are now in a new plot.

```
create-new-plot X .

set-plot-option . A Y 1 T N<sub>ppt</sub> [m<sup>-3</sup>] $ y-axis title

set-plot-option . A Y 1 Y log $ Log scale on y-axis

set-plot-option . S N B NUM_PREC$CEMENTITE_P0 %s

set-plot-option . S N B NUM_PREC$FCC_A1#01_P0 %s

set-plot-option . S M 0 Cementite $ Rename series in plot -> "Cementite"

set-plot-option . S M 1 NbC $ Rename series in plot -> "NbC"
```

The final of the four plots shows the mean precipitate radius.

```
create-new-plot X .

$ Plotting the mean radius

set-plot-option . A Y 1 T R<sub>mean</sub> [m] $ y-axis title

set-plot-option . A Y 1 Y log $ Logarithmic scale on y-axis

set-plot-option 4 S N B R_MEAN$CEMENTITE_P0 %s

set-plot-option 4 S N B R_MEAN$FCC_A1#01_P0 %s

set-plot-option 4 S M 0 Cementite $ Rename series in plot -> "Cementite"

set-plot-option 4 S M 1 NbC $ Rename series in plot --> "NbC"
```

Major gridlines are switched on for both x- and y-axes of all plots. Here the plots are referred to their number, starting from 1.

```
set-plot-option 1 G M X Y

set-plot-option 1 G M Y Y

set-plot-option 2 G M X Y

set-plot-option 2 G M Y Y

set-plot-option 3 G M X Y

set-plot-option 3 G M Y Y

set-plot-option 4 G M X Y

set-plot-option 4 G M Y Y
```

The plots are arranged so that they occupy two columns:

```
set-gui-window-property . N 2
```


A new GUI window of type p5 is created for the first histogram:

```
new-gui-window p5
```

The default x-axis is set up, with the scaling factor used to give plotting in nanometres rather than metres.

```
set-gui-window-property . S U Y
set-gui-window-property . S T Precipitate radius [nm] $ x-axis title
set-gui-window-property . S F 1e9 $ Multiplication [f]actor
```

A [n]ew [s]eries showing the [p]recipitate distribution of the “cementite_p0” phase is plotted:

```
set-plot-option . S N P CEMENTITE_P0
```

Options controlling the histogram are then set.

```
set-plot-option . H N 20 $ [n]umber of [h]istogram classes set to 20
set-plot-option . T Cementite precipitate distribution $ plot title
set-plot-option . A Y 1 T Number density of precipitates [m<sup>-3</sup>]
set-plot-option . L N $ [N]o legend box
```

The second histogram, for NbC precipitates, is set up similarly.

```
new-gui-window p5

set-gui-window-property . S U Y $ Use default x-axis
set-gui-window-property . S T Precipitate radius [nm] $ x-axis title
set-gui-window-property . S F 1e9 $ Multiplication [f]actor

set-plot-option . S N P FCC_A1#01_P0

set-plot-option . H N 20 $ number of classes
set-plot-option . T NbC precipitate distribution $ plot title
set-plot-option . A Y 1 T Number density of precipitates [m<sup>-3</sup>]
set-plot-option . L N
```

RUNNING THE CALCULATION

We first save the workspace setup as it before the calculation. This enables us to easily revert to this pre-calculation state if necessary.

```
save-workspace Tutorial_19_setup
```

An isothermal calculation can be carried out as follows. This can be useful as a preliminary calculation to check that everything is working.

An end-time for the simulation is first set:

```
set-simulation-parameter E 7200 $ Simulation end tim[e] in s
```

Then, the temperature control of the simulation is set to be [I]sothermal and the required temperature specified.

```
set-simulation-parameter T I 600
```

A further line is added to specify that this temperature is in Celsius.

```
set-simulation-parameter P Y $ Tem[p]erature in Celsius
```

The calculation can then be executed using:

```
start-precipitate-simulation
```

When this has been successfully carried out, the line specifying isothermal temperature control should be commented out by prepending a dollar sign so that it looks as shown:

```
$set-simulation-parameter T I 600
```

The temperature control is instead set to be governed by the [h]eat treatment “sample_ht” with a maximum temperature step of 10:

```
set-simulation-parameter T H sample_ht 10
```

Again, the simulation is started using:

```
start-precipitate-simulation
```

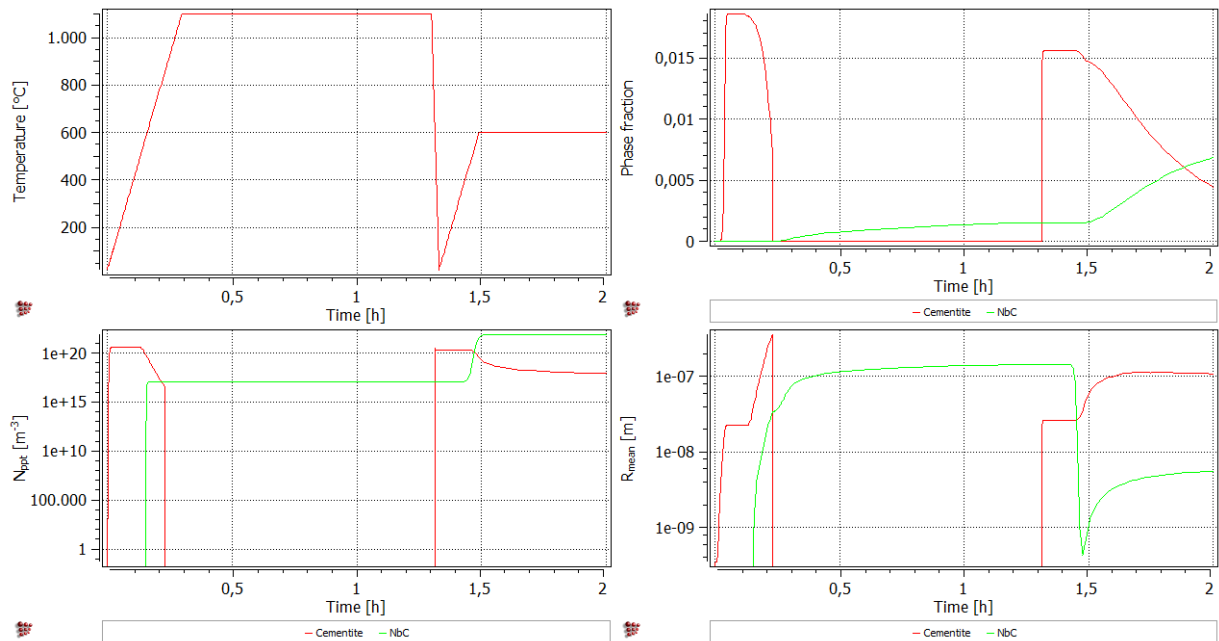
When the calculation is over, the workspace can be saved using:

```
save-workspace Tutorial_19
```

In addition, we can export whole frames or individual plots:

```
export-frame-to-file 2 N frame.png
export-frame-to-file 3 N T19_histo_cementite.png
export-plot-to-file 4 N T19_Rmean
```

The x-y plot window should look as follows after the calculation:



T20: SIMULATING GRAIN GROWTH

This tutorial was tested on

MatCalc version 6.00 rel 1.000

license: free

database: mc_fe.tdb; mc_fe.ddb

CONTENTS

- Single-class model for grain growth
- Multi-class model for grain growth
- Grain growth with pinning and solute drag

SETTING UP THE SYSTEM

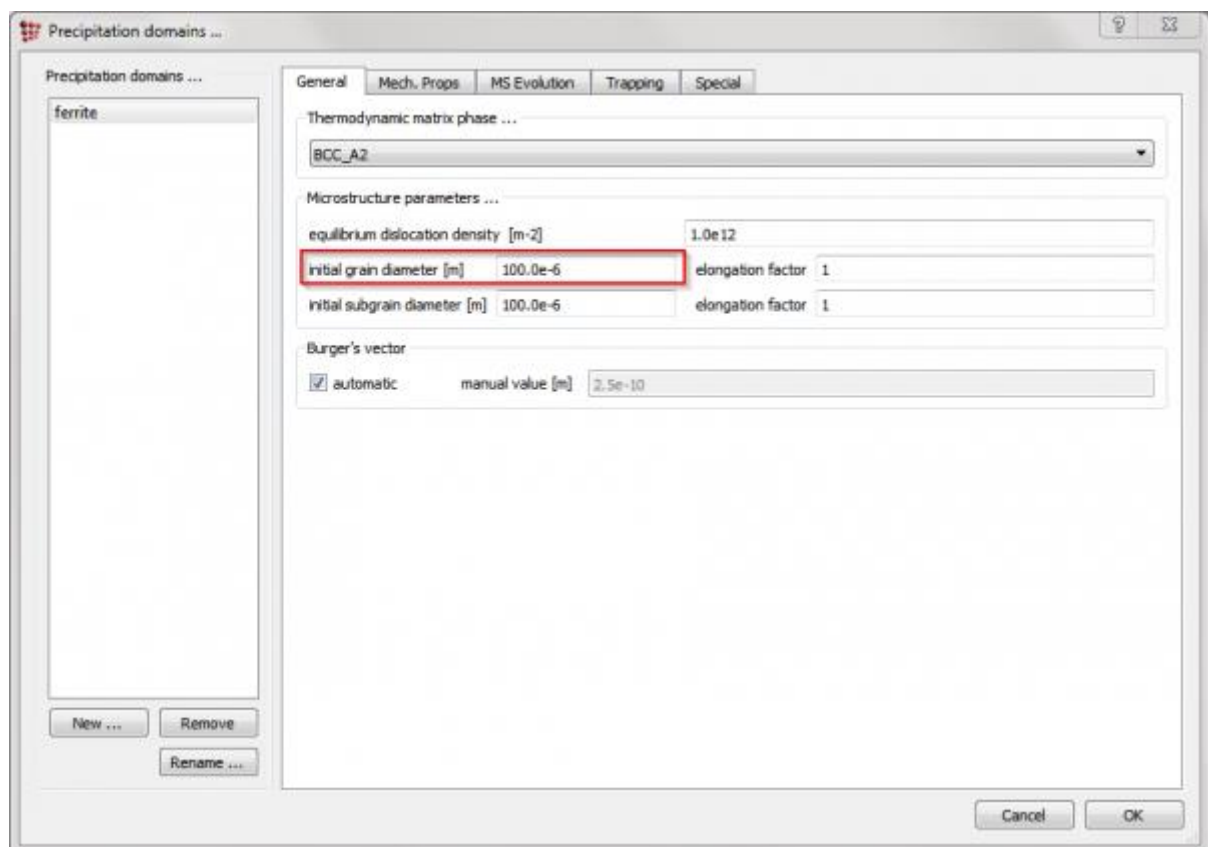
From the database `mc_fe.tdb`, select the element `FE` and the phase `BCC_A2`. Read in the mobility database `mc_fe.ddb`. Create a precipitation domain named 'ferrite' associated with the phase `BCC_A2`.

SINGLE-CLASS GRAIN GROWTH MODEL

We start with the simplest possible scenario for grain growth: a single-phase, pure metal with no solutes or precipitates present to retard grain growth.

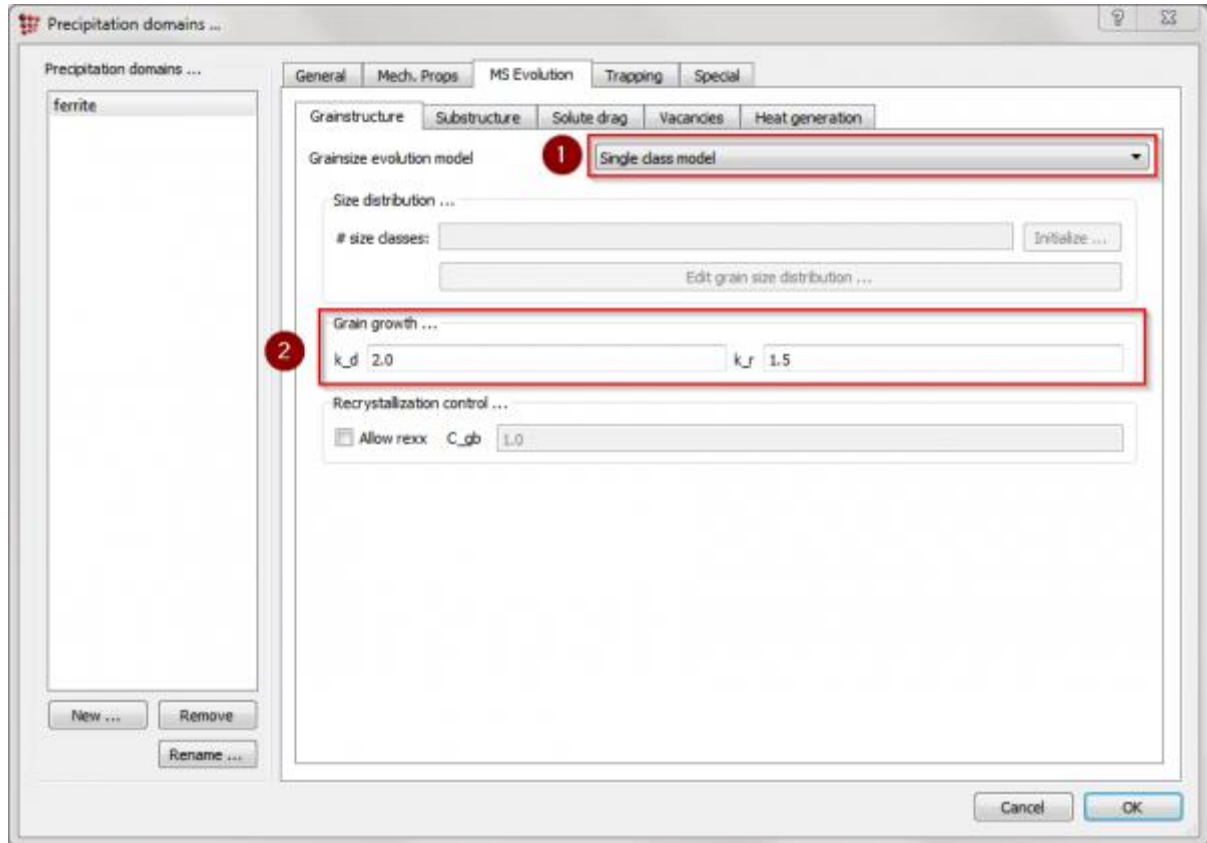
There are two parts to the setting-up of the simulation, both in **Precipitation domains**. (Note that a *precipitation domain* must be set up and configured for the grain growth simulation, even if no precipitation is taking place.)

In the **general** tab, specify the **Initial grain size**. In this example we will leave this at the default value:



Then, go to the **MS Evolution** tab and select the **Grainstructure** sub-tab. By default, the evolution model for grain size is set to **None - no evolution**. This is the option that has been used in all kinetic simulations so far; the grain size, as well as other microstructural parameters such as dislocation density, has been taken as constant. Instead, set this to **Single class**

model (No. (1) in the diagram below). A set of options will appear as shown in the diagram below. For the single-class model, we are only concerned with the parameters marked with the number (2).



The model implemented in MatCalc is described in ¹⁾. The rate of change of the diameter D of the grains as a function of time given by:

$$\frac{dD}{dt} = M \cdot (P_d - P_r)$$

where M is the mobility of the grain boundaries and P_d and P_r are the driving force and the retarding pressure on the grain boundaries, respectively.

M is given by an Arrhenius expression:

$$M = M_0 \exp\left(\frac{-Q}{RT}\right)$$

where M_0 is a pre-exponential factor, Q is the activation energy of the mobility, T is the absolute temperature, and R the gas constant.

The driving force P_d depends on the grain boundary energy γ_g and the grain diameter D :

$$P_d = k_d \left(\frac{\gamma_g}{D} \right)$$

and the retarding force due to pinning by a volume fraction f_v of particles with diameter d is given by:

$$P_r = k_r \left(\gamma_g \cdot \frac{f_v}{d} \right)$$

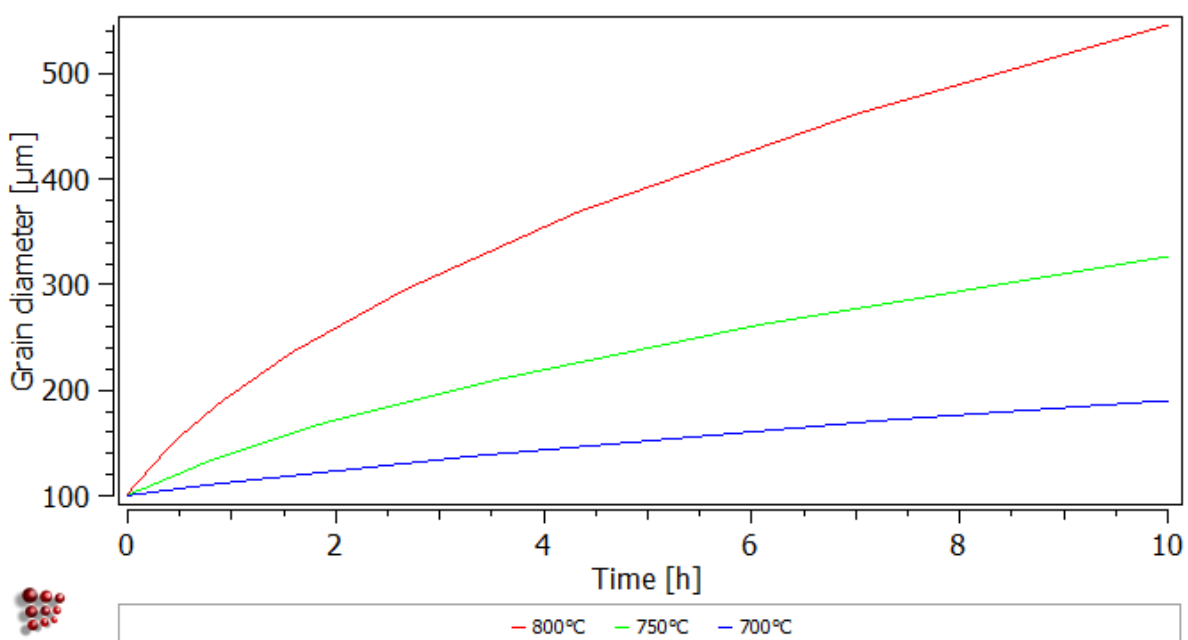
The terms k_d and k_r are the constants that appear in the dialogue box above.

Accept these default settings for the present.

Using **Calc > precipitation kinetics**, set up an isothermal simulation with an end-time of 36000 s and a temperature of 800°C. Click on Go. The simulation will be over very rapidly compared to precipitation simulations.

Create a plot of type p1. In the **variables** window, find the section entitled **prec domain struct sc** (single class) and expand to show **GD\$***. Expand this one step further to show **GD\$ferrite**, and drag this to the plot window. Change the (default x-axis label to read **time [h]** and modify the scaling factor to **1/3600**. Change the y-axis title to **Grain diameter [x10⁻⁶m]** and modify the scaling factor to **1/1e-6**.

Label the existing series **800°C**, duplicate and lock it and repeat the calculation for 750°C and 700°C to give curves as shown:



CHANGING THE MODEL PARAMETERS

Changing k_r will not modify the results in the present case, because we have not yet set up any mechanism to retard the grain growth. However, as would be expected from the equations above, changing k_d to a lower value gives a smaller grain size at the same time, all else being equal.

Experiment also with different initial grain diameters. If the initial grain diameter is reduced, the curve moves downwards to smaller grain sizes for a given time and temperature.

1) M. Rath & E. Kozeschnik, "Coupled grain growth and precipitation modeling in multi-phase systems", Materials Science Forum Vol. 753 (2013) pp 357-360

T21: STRAIN INDUCED PRECIPITATES

This tutorial was tested on

MatCalc version 6.00 rel 0.047

license: free

database: mc_fe.tdb; mc_fe.ddb

CONTENTS

- Effect of volumetric misfit on precipitation kinetics
- Introduction of deformation into the thermo-mechanical treatment
- Effects of the applied deformation on the precipitation kinetics

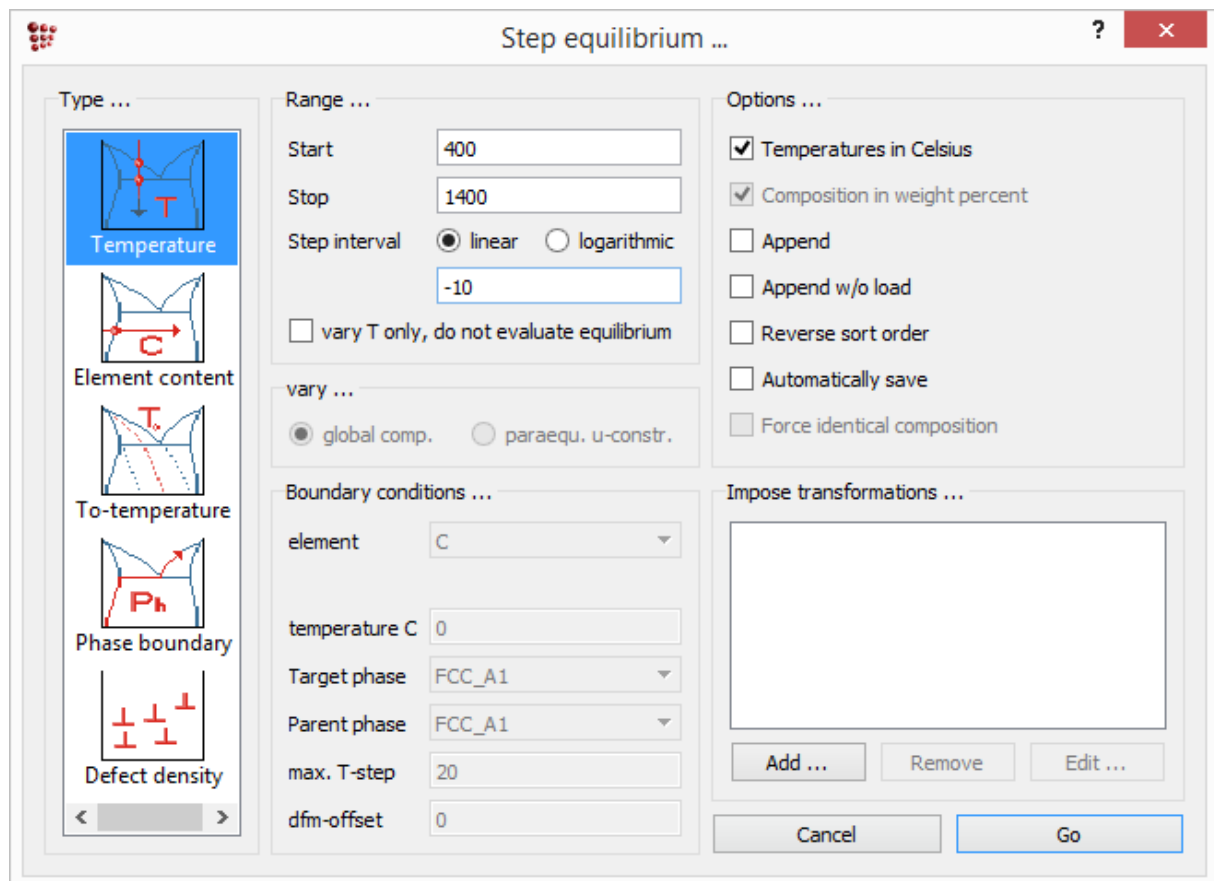
Deformation process influences the microstructure of the alloy. One of the effects is the occurrence of the strain induced precipitates. This tutorial demonstrates how the deformation processes can be included in the simulation of the processed material. Moreover, the effects of the deformation on the precipitation kinetics are demonstrated and discussed.

SETTING UP THE SYSTEM

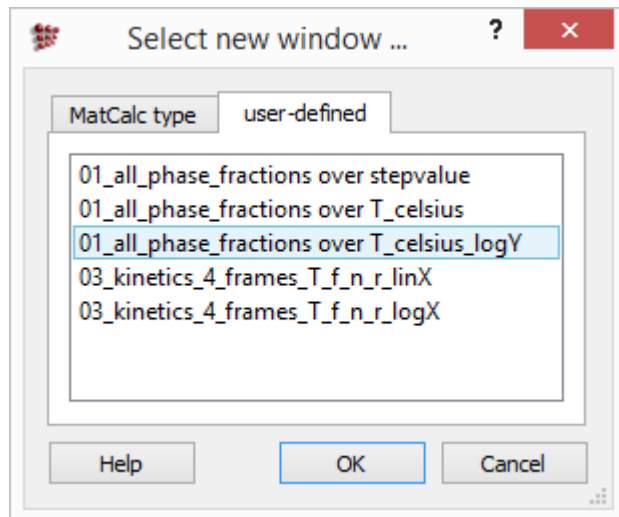
Create a new workspace and open the '**mc_fe.tdb**' database. Select the elements '**Fe**', '**Nb**' and '**C**', together with the phases '**BCC_A2**', '**FCC_A1**' and '**Cementite**'. Click on 'Read' instead of 'Read & Close', as the subsequent step is to read the diffusion database in this window. Select '**Diffusion data**' on the left side and read the '**mc_fe.ddb**' database. Enter the composition of **0.2 wt.% C** and **0.04 wt.% Nb**. Click on '**Set automatic startvalues**' and calculate an equilibrium at the initial 1000°C.

PHASE SOLUBILITIES

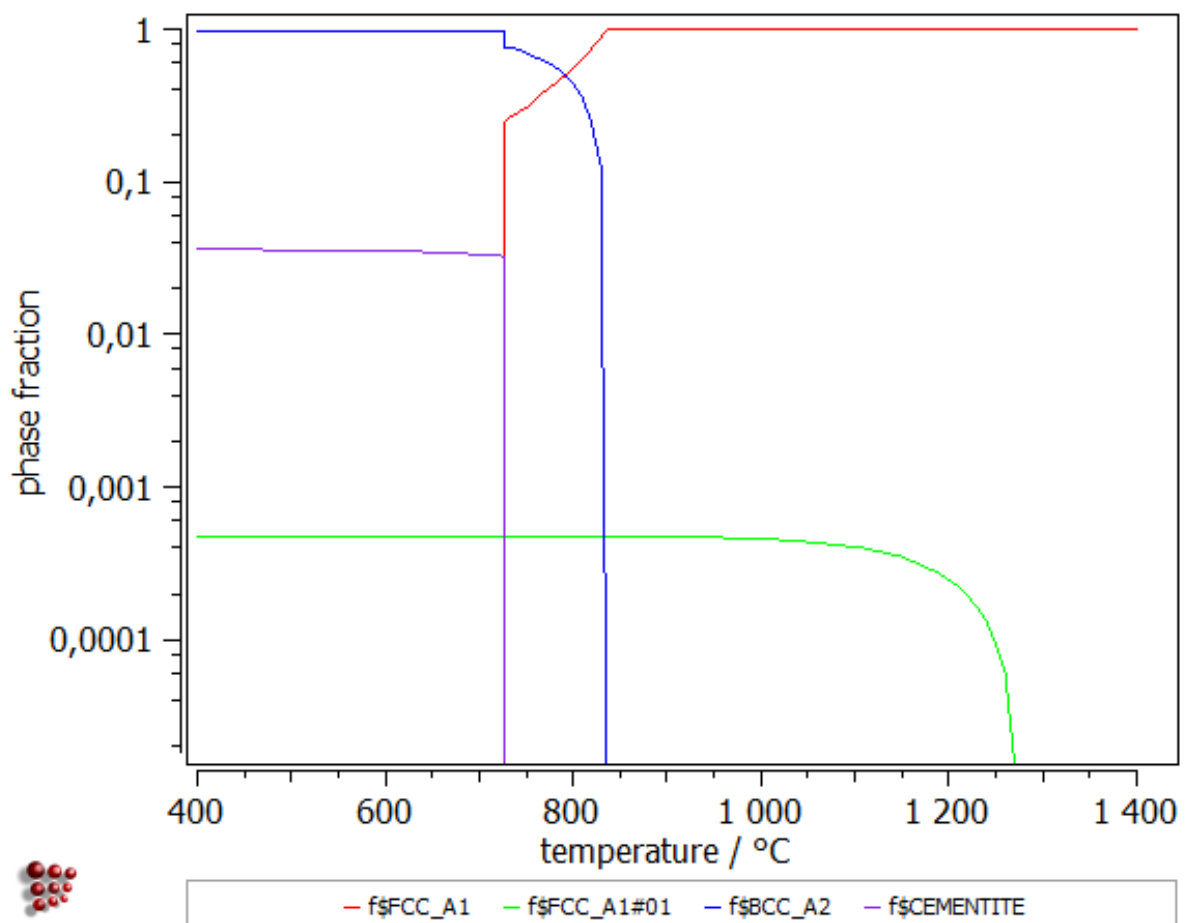
In order to have some insight into the system equilibria, perform a stepped equilibrium calculation. In '**Stepped equilibrium**' window select the temperature range of 400-1400°C with the step of 10°C. Click on '**OK**'



The phase fractions can be plotted by calling the appropriate user-defined window. In '**View**' → '**Create new window**', select the 'user defined' tab. There, select '**01_all_phase_fractions over T_celsius_logY**' and click on '**OK**'.



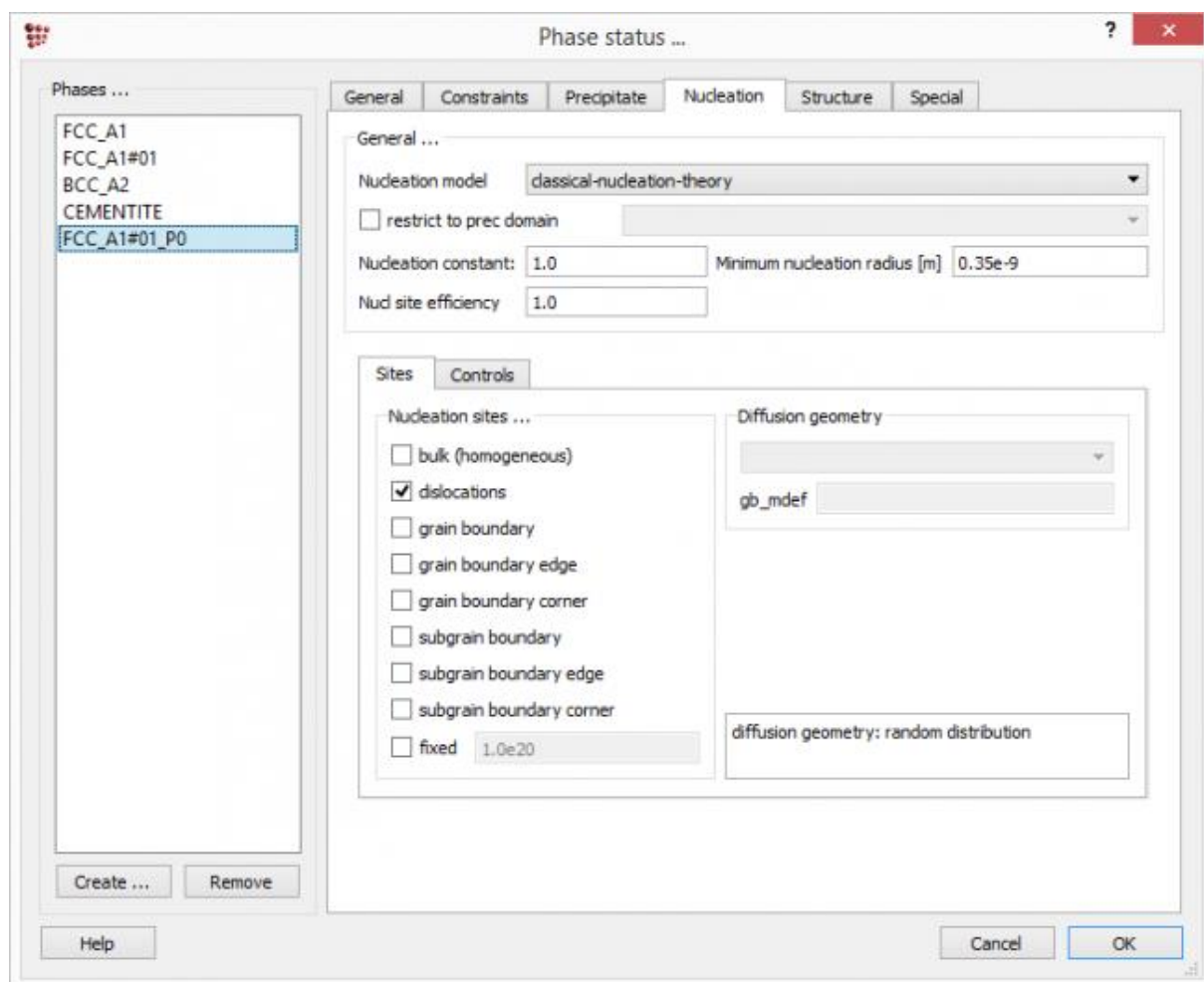
This will result in the plot looking like the one shown below. From this diagram it can be concluded that NbC precipitates below 1300°C and the ferrite will form below 850°C.



PRECIPITATION DOMAINS AND PHASES

Next, create a precipitation domain called '**austenite**' in the 'Precipitation domains ...' window. Select **FCC_A1** as the **thermodynamic matrix phase**.

Now, define the precipitate phase settings in '**Phase status**' window. Select '**FCC_A1#01**' and click on '**Create**' and '**precipitate (_Pnn)**'. In 'Nucleation' → 'Sites' set 'dislocations' as nucleation sites (and remove the checkmark from 'bulk').



THERMO-MECHANICAL TREATMENT

The last step before the initial kinetics simulation is the definition of the thermo-mechanical treatment. In '**Global**' → '**Thermo-mech. treatments ...**' create a new treatment with the name '**cooling**'. Next, create a segment in which the austenite domain will be cooled from **1300°C** to **750°C** with **1°C/s** cooling rate.

Edit t/m treatment segment ...

General MS Evolution

Temperature ...

Start temperature: 1300

Ramp control ...

End temperature & Heat/Cooling Rate

End temperature: 750

Heat/Cooling Rate: -1

Delta-Time: 550

Accumulated strain: 0

Store Interval ...

Intervals: 25 ☐ lin

log scale factor: 1.1 ☒ log

☐ reset store counter

Precipitation Domain ...

☐ inherit from previous segment

☒ select austenite

Comment Pre-Segment Script Post-Segment Script

Clear

0 +

Cancel OK

Edit thermo-mechanical treatments ...

Available treatment ...

cooling

New ... Rename ... Duplicate

Remove HT Write ... Read ...

Preview ...

1300
1200
1100
1000
900
800
700

0 100 200 300 400 500

Preferences ...

Time axis scaling:

☒ Linear

☐ Logarithmic

Minimum time: 0

Maximum time: 528

Data ...

Seg	Start T	End T	T dot	Delta t	acc eps	Total t	#Intv.	Lin/Log	Prec. dom	eps_dot	res_va	res_rexx	break_up	release
0	1300	750*	-1*	550	0	550	25	log	austenite	0.0	-	-	-	-

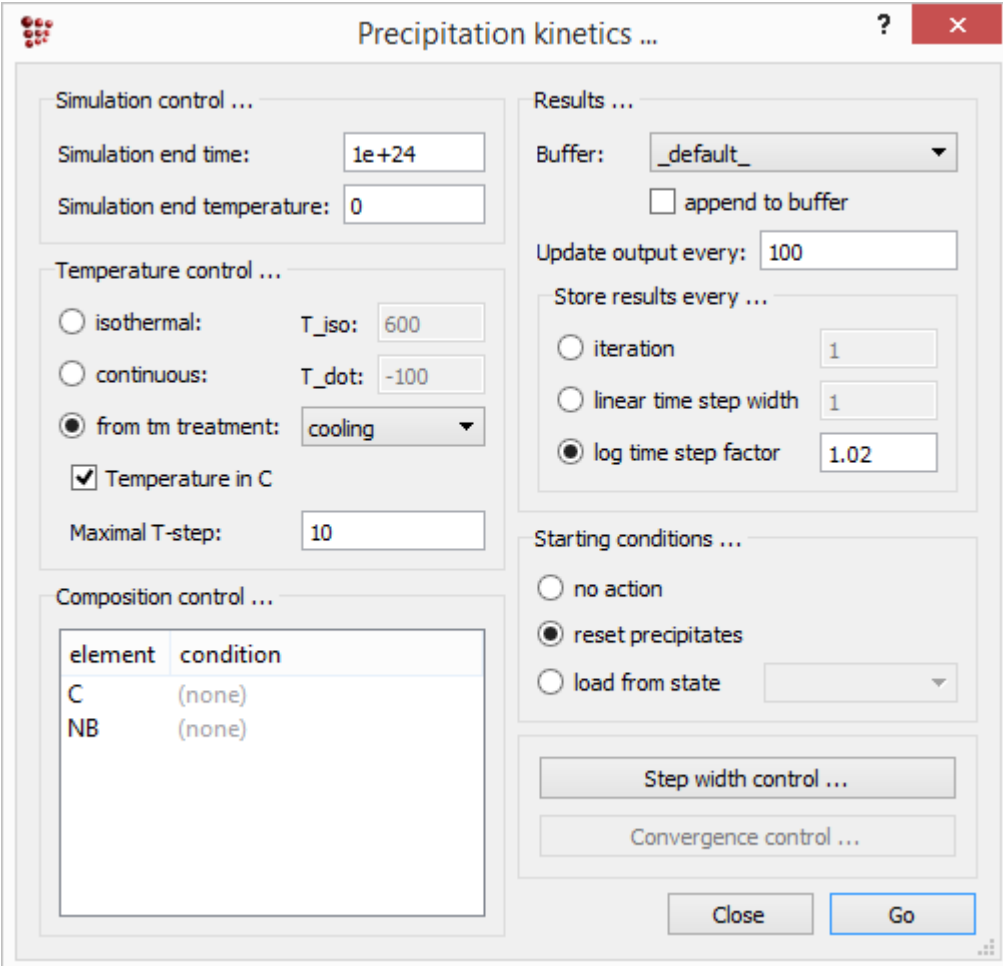
< >

New segment Insert segment Remove Edit

Cancel OK

KINETICS SIMULATION OF SIMPLE COOLING PROCESS

With all the setup procedures done, perform the kinetics simulation. Click on '**Calc**' → '**Precipitation kinetics**'. Select the '**cooling**' treatment in the '**Temperature control ...**' area and click on '**Go**'.



Precipitation kinetics ...

Simulation control ...

Simulation end time:

Simulation end temperature:

Temperature control ...

☐ isothermal: T_{iso}:
☐ continuous: T_{dot}:
☒ from tm treatment:
☒ Temperature in C
 Maximal T-step:

Composition control ...

element	condition
C	(none)
Nb	(none)

Results ...

Buffer:
☐ append to buffer

Update output every:

Store results every ...

☐ iteration
☐ linear time step width
☒ log time step factor

Starting conditions ...

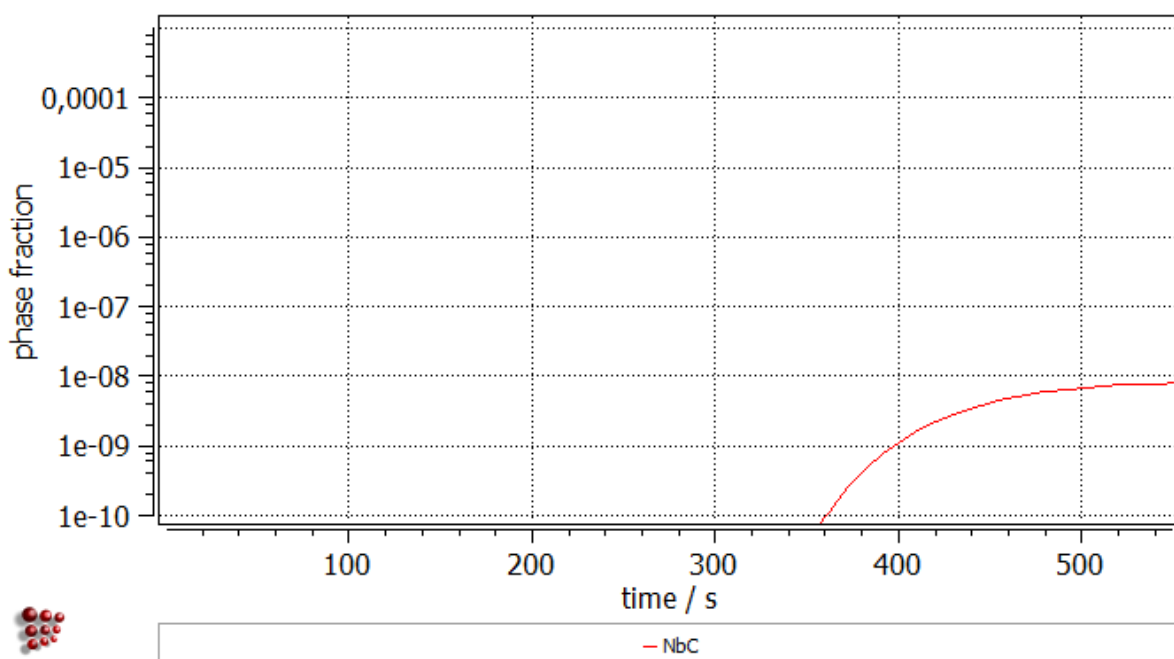
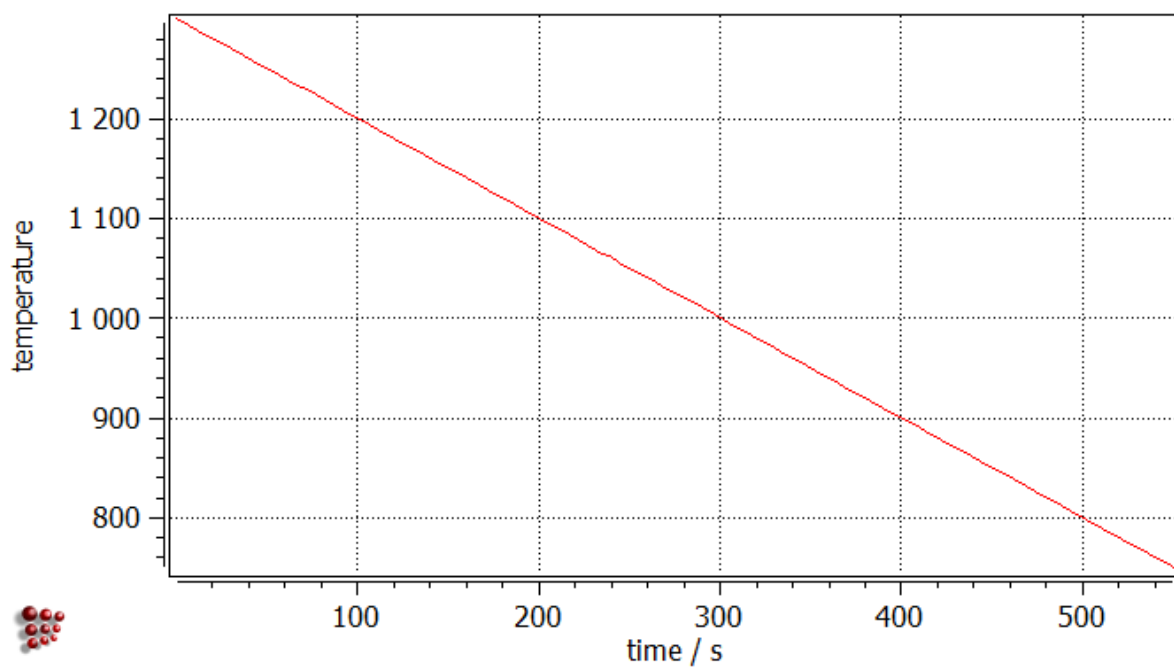
☐ no action
☒ reset precipitates
☐ load from state

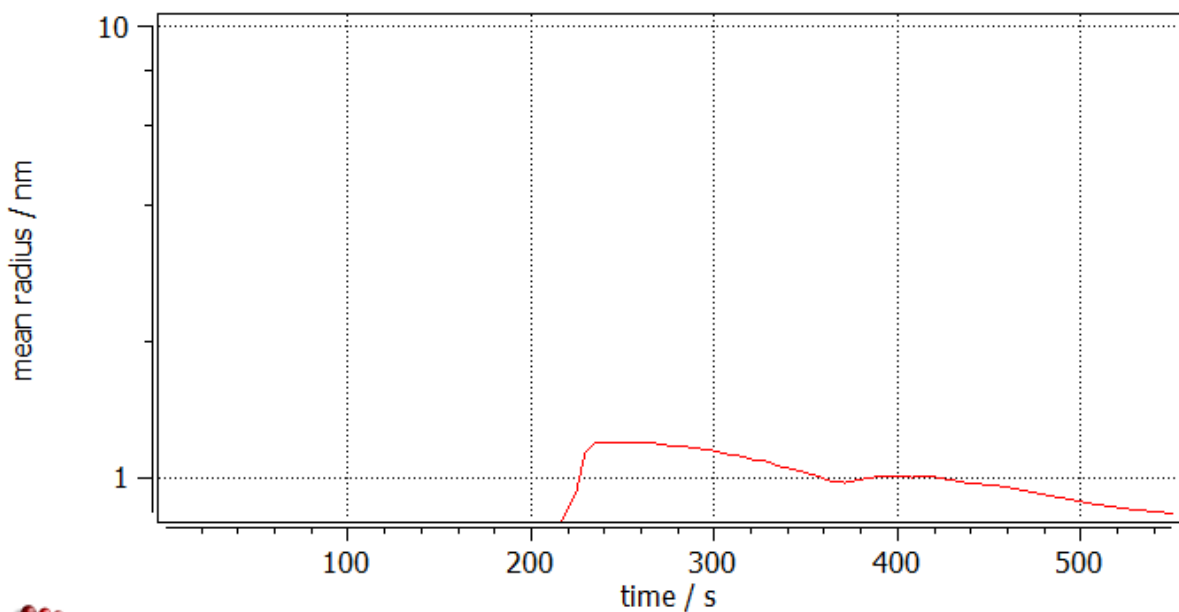
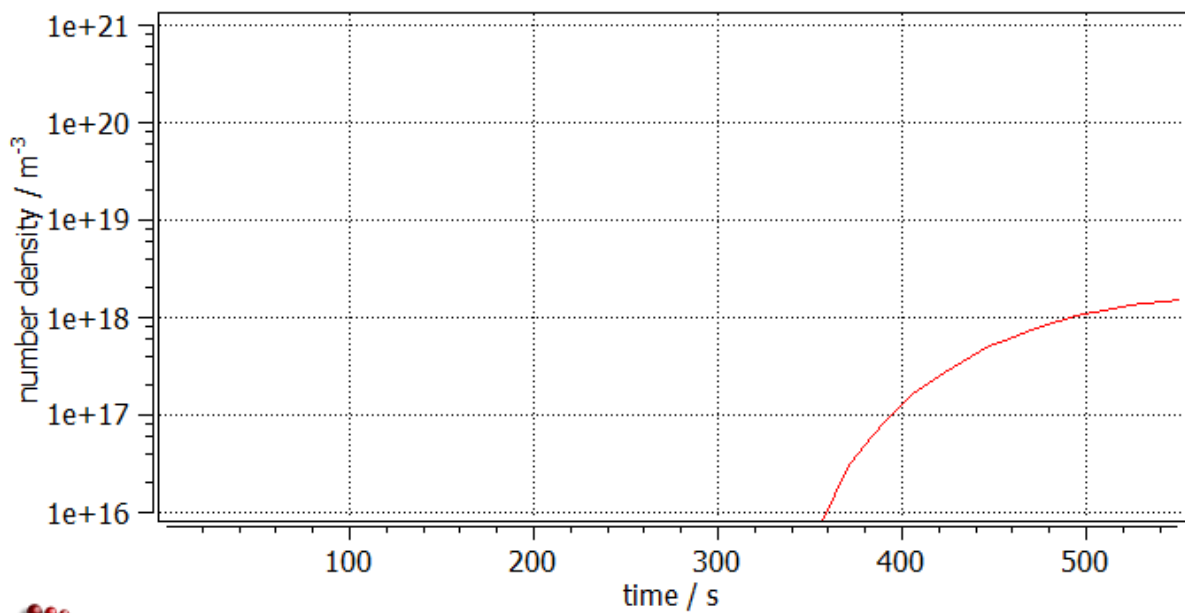
Step width control ...

Convergence control ...

Close Go

Once the calculation is completed, use the 'user defined plots' for visualizing the phase fraction, number density and mean radius evolution of the precipitates, as well as the temperature profile. Click on '**View**' → '**Create new window**', select the '**user-defined**' tab and choose the last entry '**03_kinetics_4_frames_T_f_n_r_linX**'. Click on '**OK**'. Set the start of the scaling range to '**1**'. The analysis of the created plots reveals a somewhat unspectacular precipitation of NbC phase after 200 s (below 1100°C) that reaches the number density of $1e18 \text{ m}^{-3}$ and stays in the nanometer range.





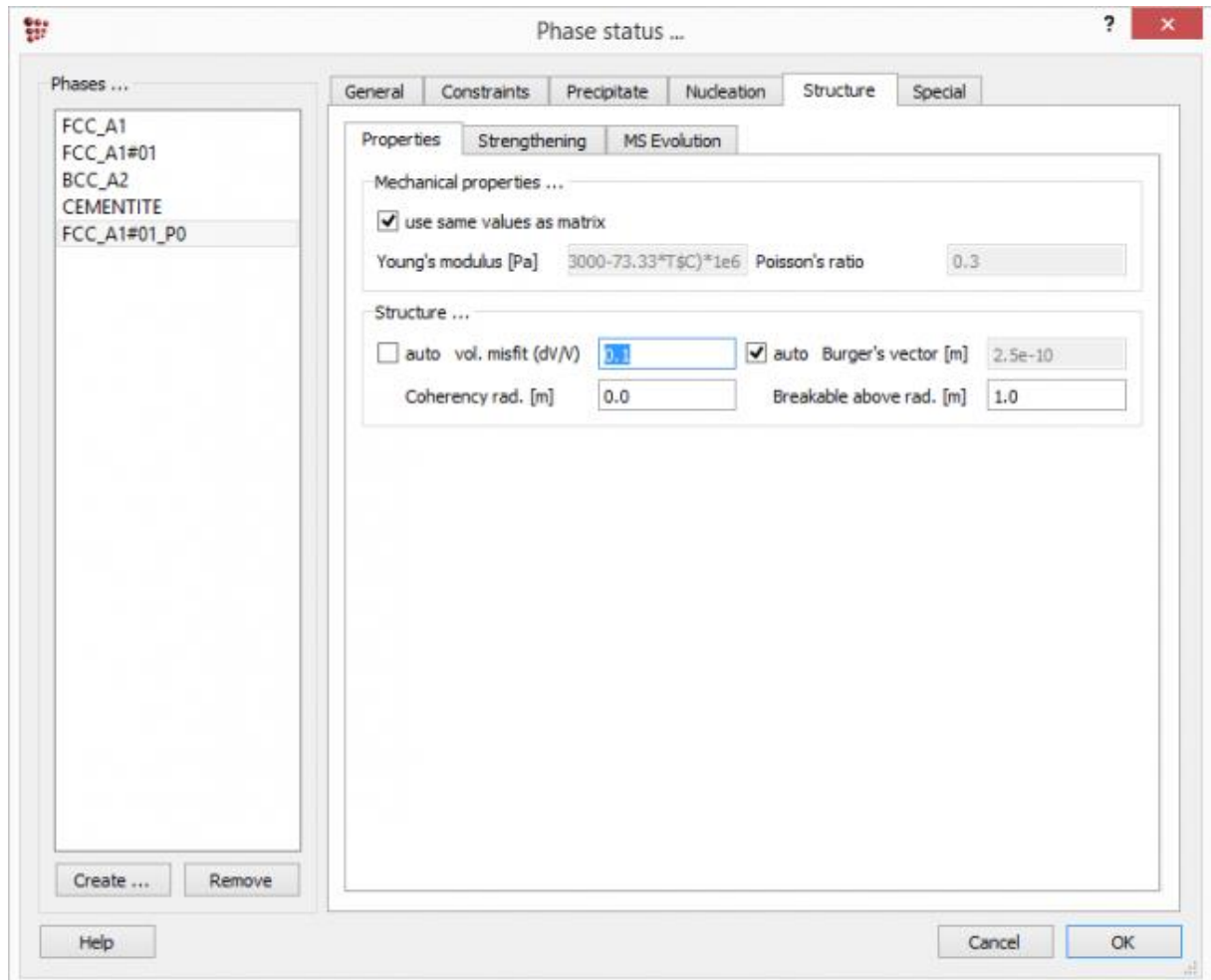
By clicking on 'Global' → 'Buffers' → 'Rename', rename the current buffer to 'Cooling'.

EFFECT OF VOLUMETRIC MISFIT

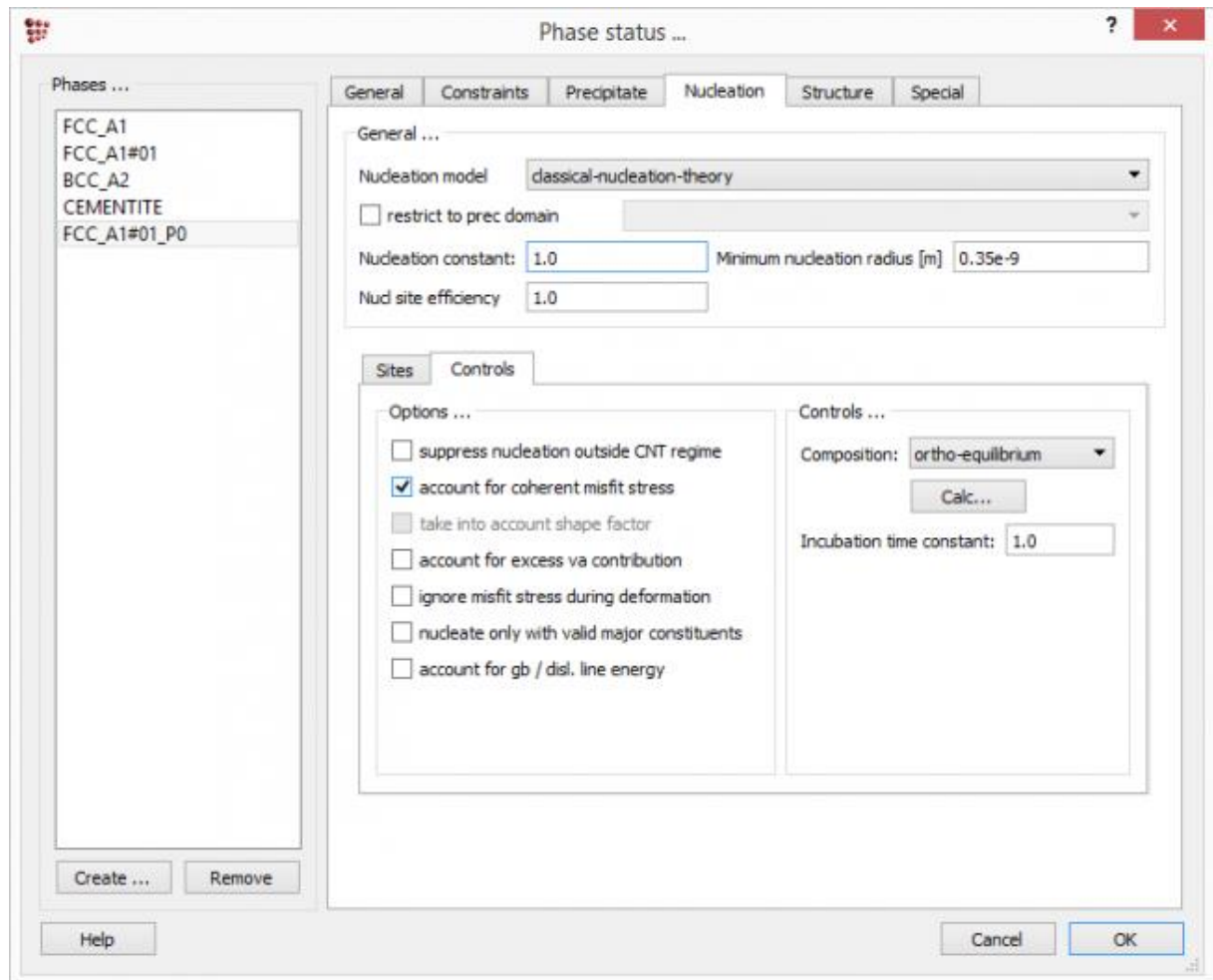
In general, the precipitates show usually different crystallographic features from the matrix phase. This will be the source of the stress acting on the precipitates within the grain which needs to be considered especially during the nucleation stage. As for now, all the simulations were performed in the previous tutorial were neglecting this factor. Now it will be

demonstrated how this effect can be introduced into the simulation and what is the effect of it.

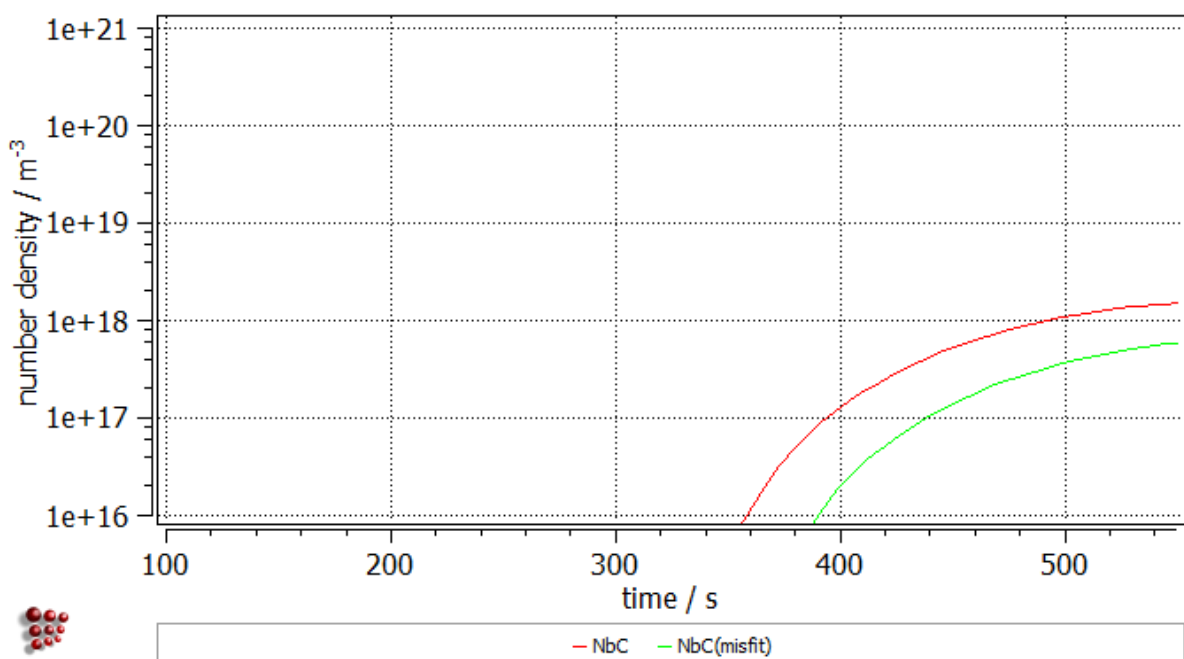
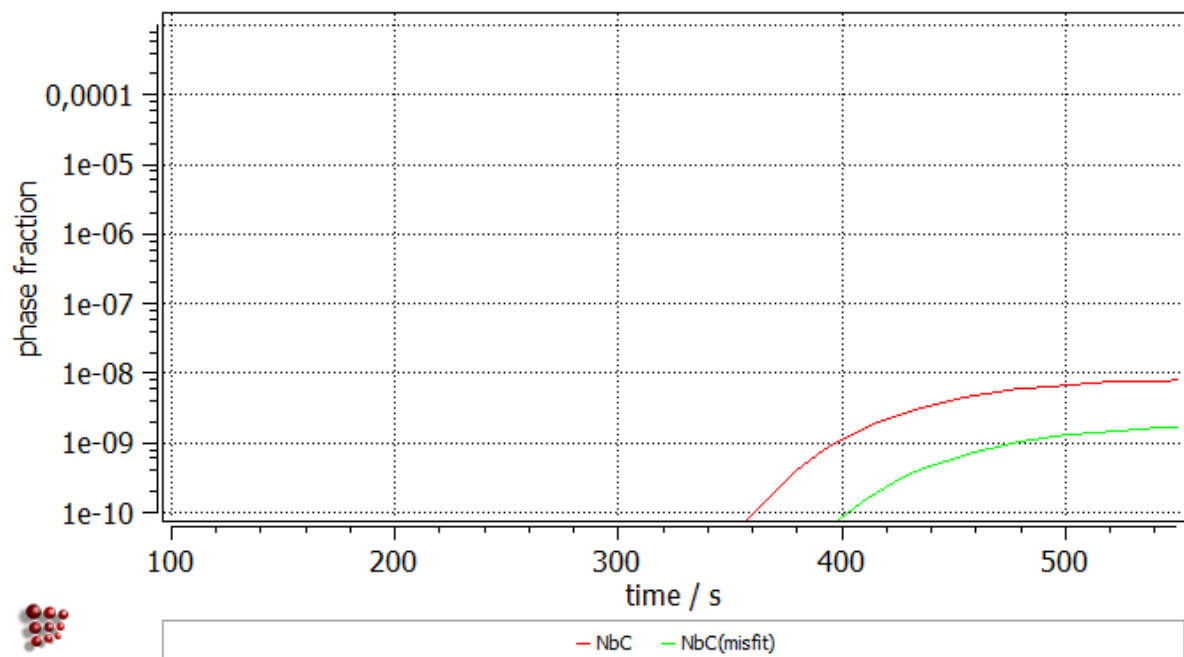
Click on '**Global**' → '**Phase status**' and select '**Structure**' tab. In the field '**vol. misfit (dV/V)**' type in the values of '**0.1**' for the precipitate phase. This represents the stress coming from the precipitate volume differing by 10% from the matrix volume.

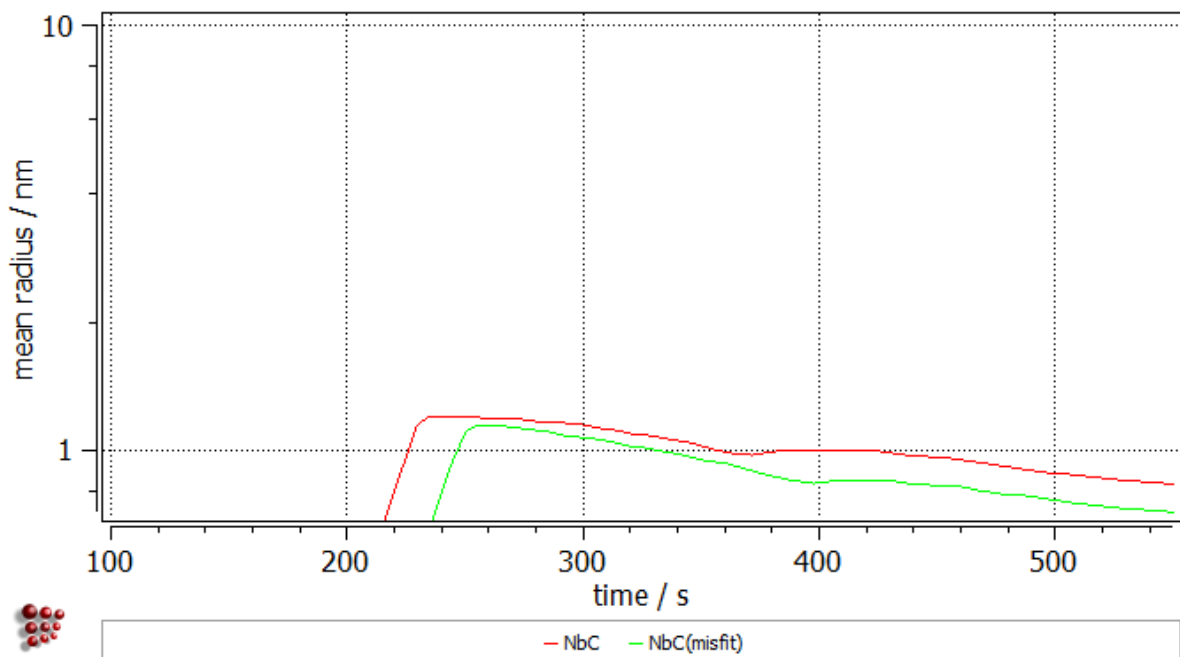


Next, in '**Nucleation**' → '**Controls**' tab put a checkmark at the 'account for coherent misfit stress' for the precipitate phase.



Click on 'OK' to close the window. Create a new buffer with the name '**Vol_misfit**'. With this buffer selected, perform again the kinetic simulation. Once the simulation is completed, duplicate and lock all series in the plots, then switch the displayed buffer to 'Vol_misfit'. As it can be noticed, the definition of the volumetric misfit decreased amount of the precipitated phase.





SIMULATION OF DEFORMATION PROCESS

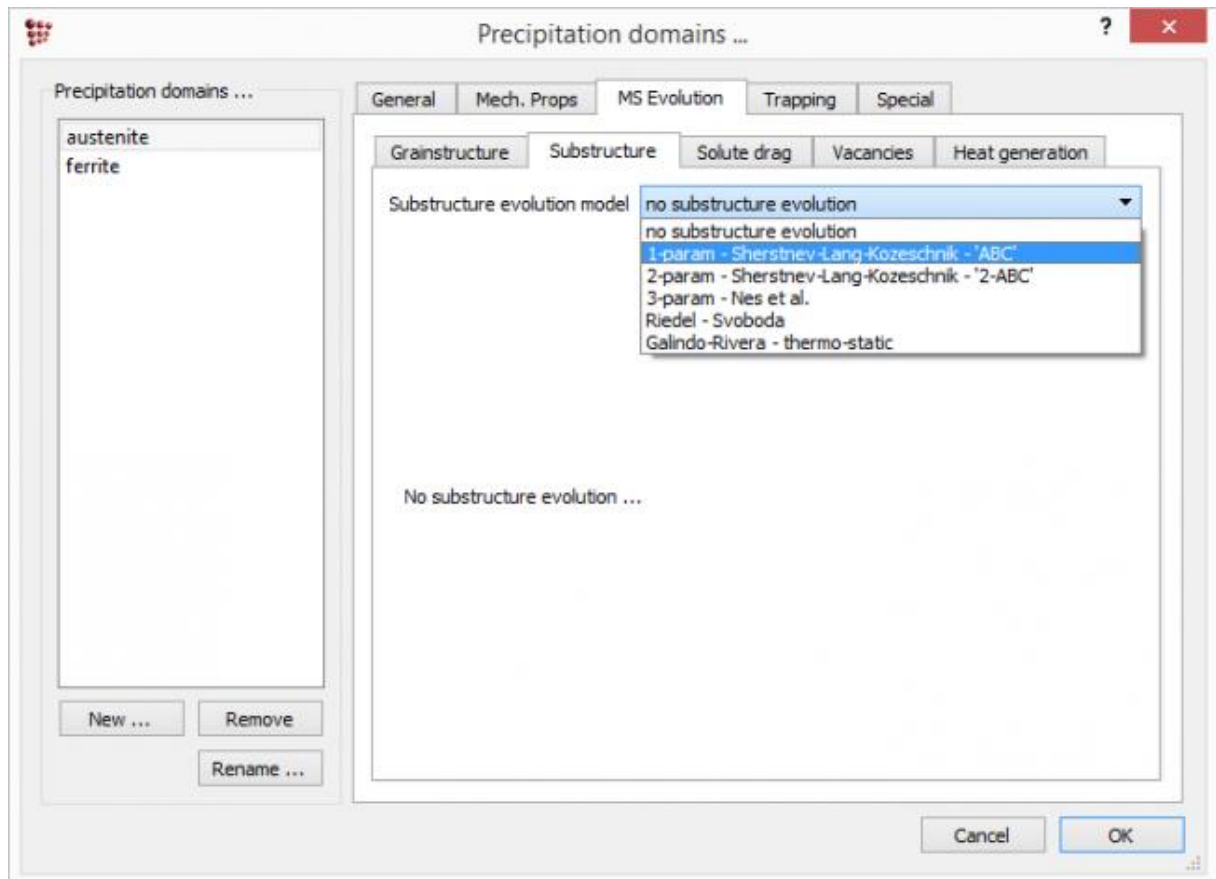
When deformation process is to be simulated, there are basically three things to be modified in the treatment:

- Activation of the dislocation density evolution model.
- Definition of the deformation rates and temperatures.
- Deactivation of the volumetric misfit effect for the nucleation during the deformation.

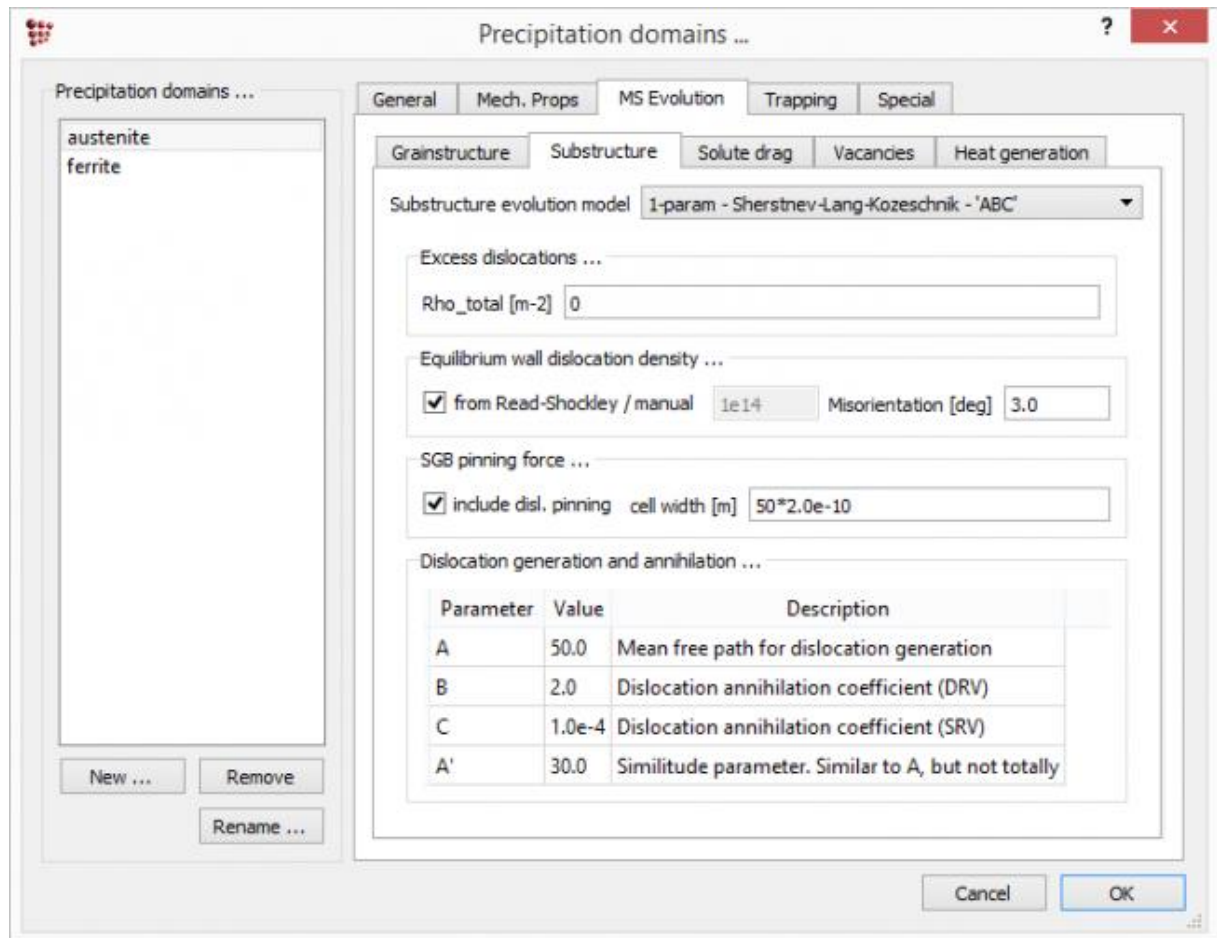
EVOLUTION OF DISLOCATION DENSITY

The deformation will change the microstructure of the alloy. Here, the change of the dislocation density by the deformation is presented.

Click on '**Global**' → '**Precipitation domains**'. The simulated deformation will be performed in the austenite region, so select austenite as a precipitation domain and switch to the '**MSEvolution**' tab. Inside, select '**Substructure**' tab and select '**1-param - Sherstnev-Lang-Kozeschnik - 'ABC''** as the model for the substructure evolution.

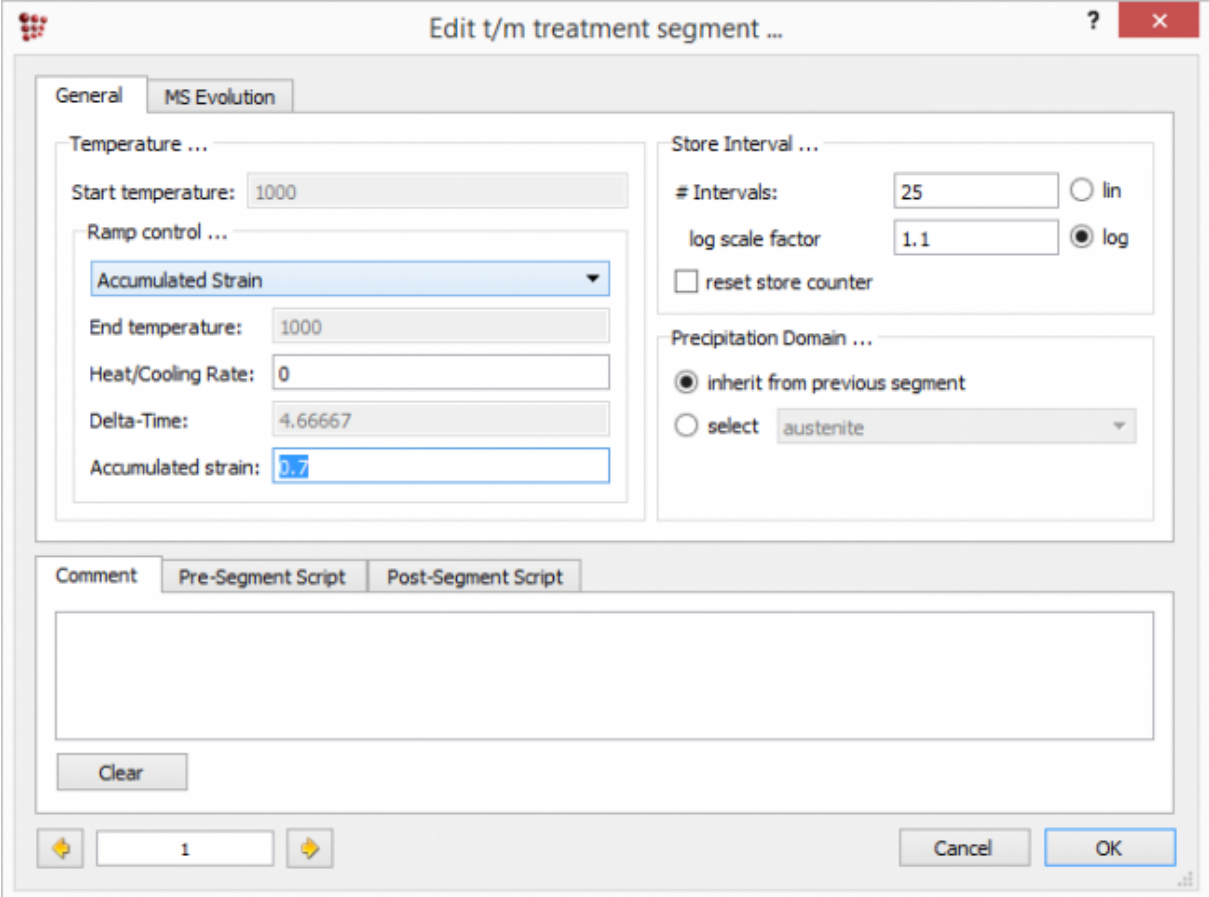


You might notice some parameters in the 'Dislocation generation and annihilation ...' section which describe the generation of the dislocations ('A'-parameter) and their annihilation during the static ('B'-parameter) and dynamic recovery ('C'-parameter). Leave all the parameters there on the default value.



THERMO-MECHANICAL TREATMENTS SETTINGS

In this simulation, three deformation runs will be represented. Click on '**Global**' → '**Thermo-mech. treatments**' and create a new treatment with the name 'deformation'. The first segment will have the starting temperature of 1300°C but the end temperature will be 1000°C with the cooling rate of 1 K/s. In the next segment, change the ramp control setting to '**Accumulated strain**' and set the '**Accumulated strain**' value to '**0.7**'.



Edit t/m treatment segment ...

General **MS Evolution**

Temperature ...

Start temperature: 1000

Ramp control ...

Accumulated Strain

End temperature: 1000

Heat/Cooling Rate: 0

Delta-Time: 4.66667

Accumulated strain: 0.7

Store Interval ...

Intervals: 25 ☐ lin

log scale factor: 1.1 ☒ log

☐ reset store counter

Precipitation Domain ...

☒ inherit from previous segment

☐ select austenite

Comment

Pre-Segment Script

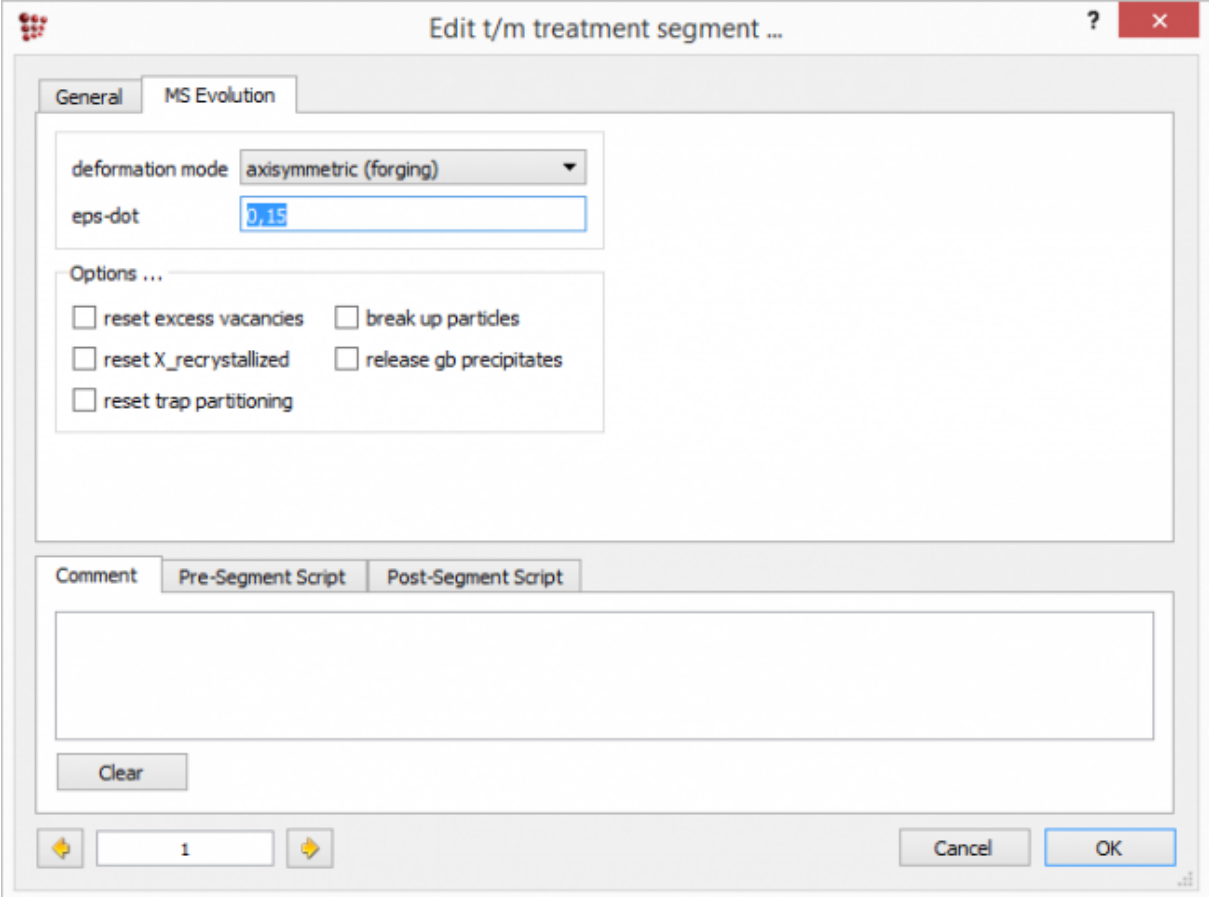
Post-Segment Script

Clear

1

Cancel OK

Afterwards, switch to the '**MS Evolution**' tab and type in the strain_rate value of '**0.15**'.



deformation mode: axisymmetric (forging)

eps-dot: 0.15

Options ...

- ☐ reset excess vacancies
- ☐ break up particles
- ☐ reset X_recrystallized
- ☐ release gb precipitates
- ☐ reset trap partitioning

Comment | Pre-Segment Script | Post-Segment Script

Clear

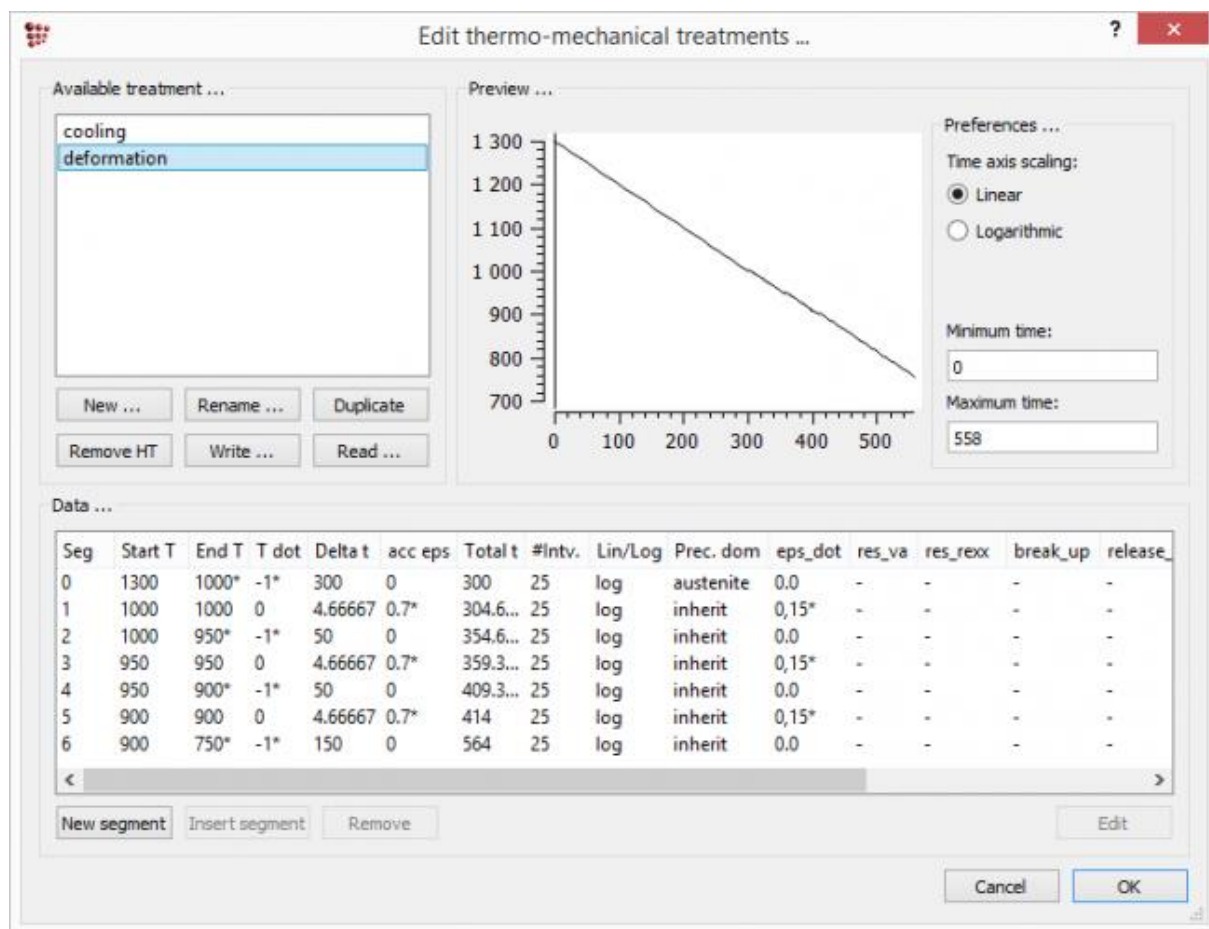
1

Cancel OK

The definition of the next segments should follow the settings below:

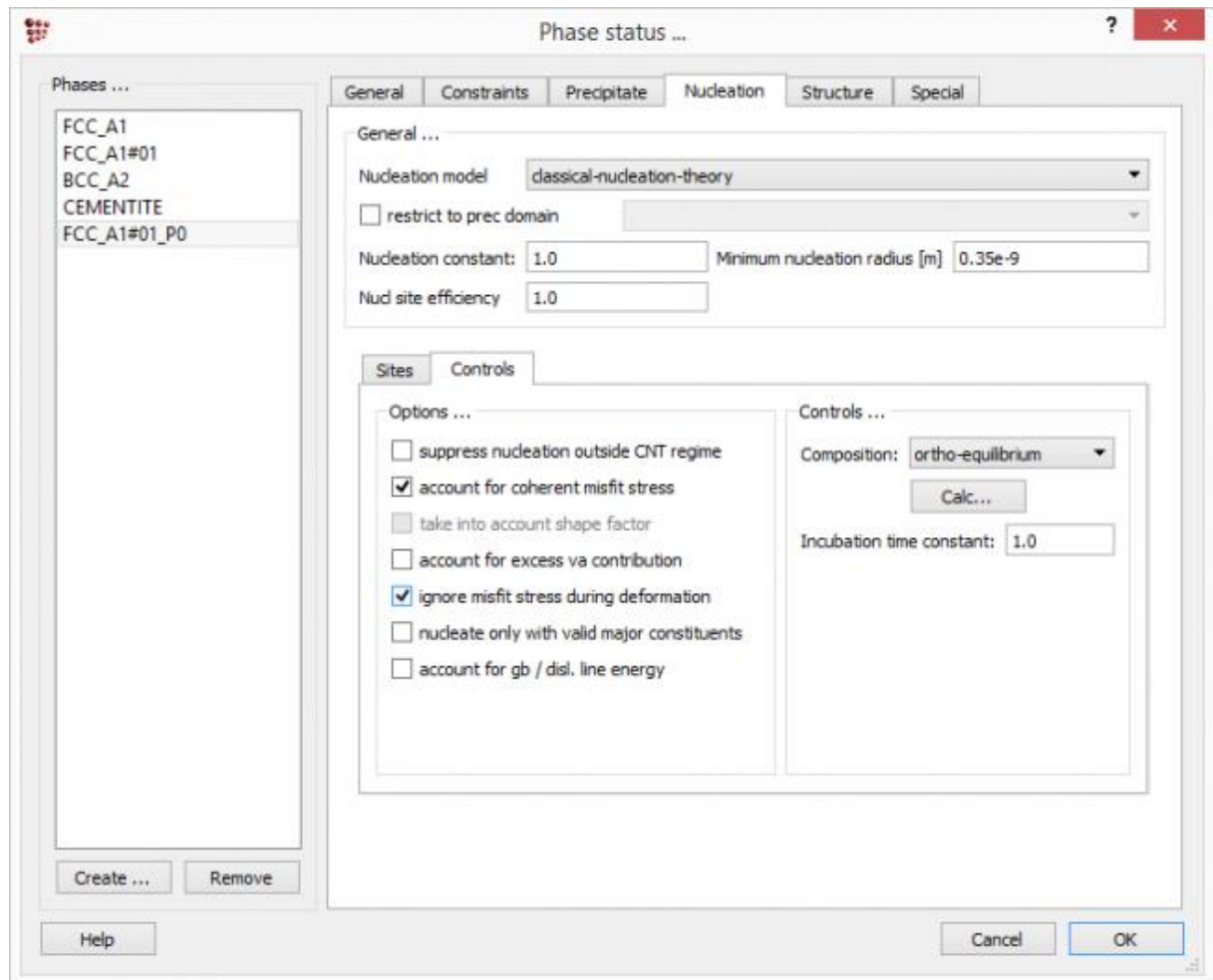
1. End temperature of 950°C with 1 K/s rate.
2. Deformation at 950°C with strain rate of 0.15 increasing the strain by 0.7.
3. End temperature of 900°C with 1 K/s rate.
4. Deformation at 900°C with strain rate of 0.15 increasing the strain by 0.7.
5. End temperature of 750°C with 1 K/s rate.

The complete treatment data are shown below.



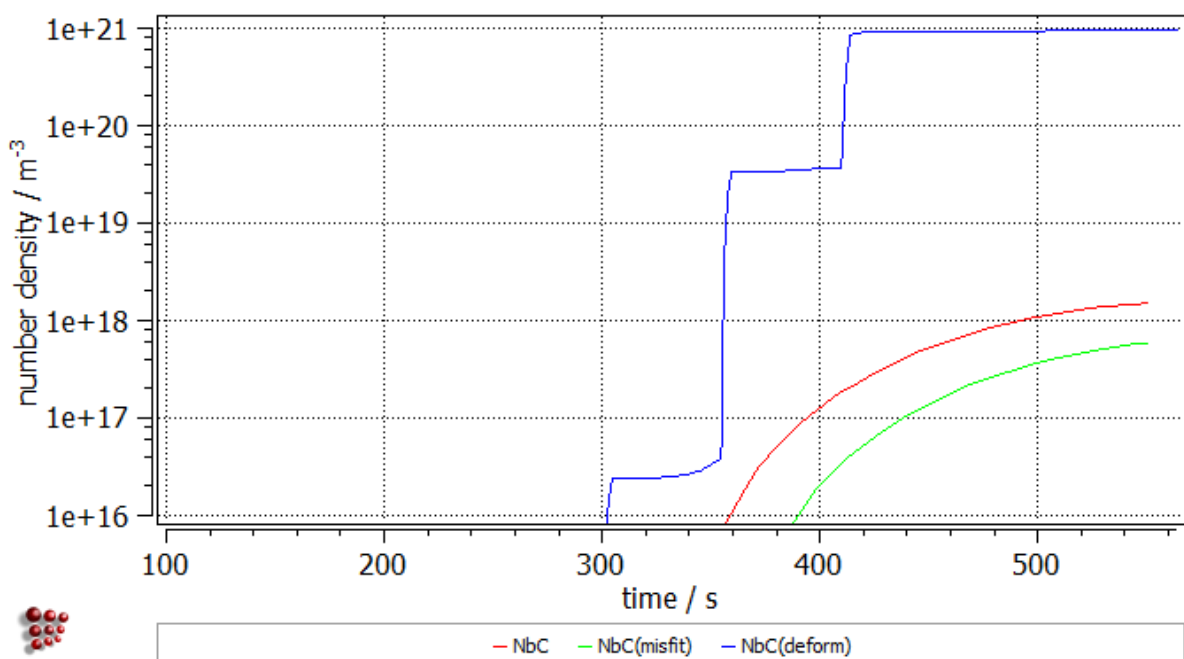
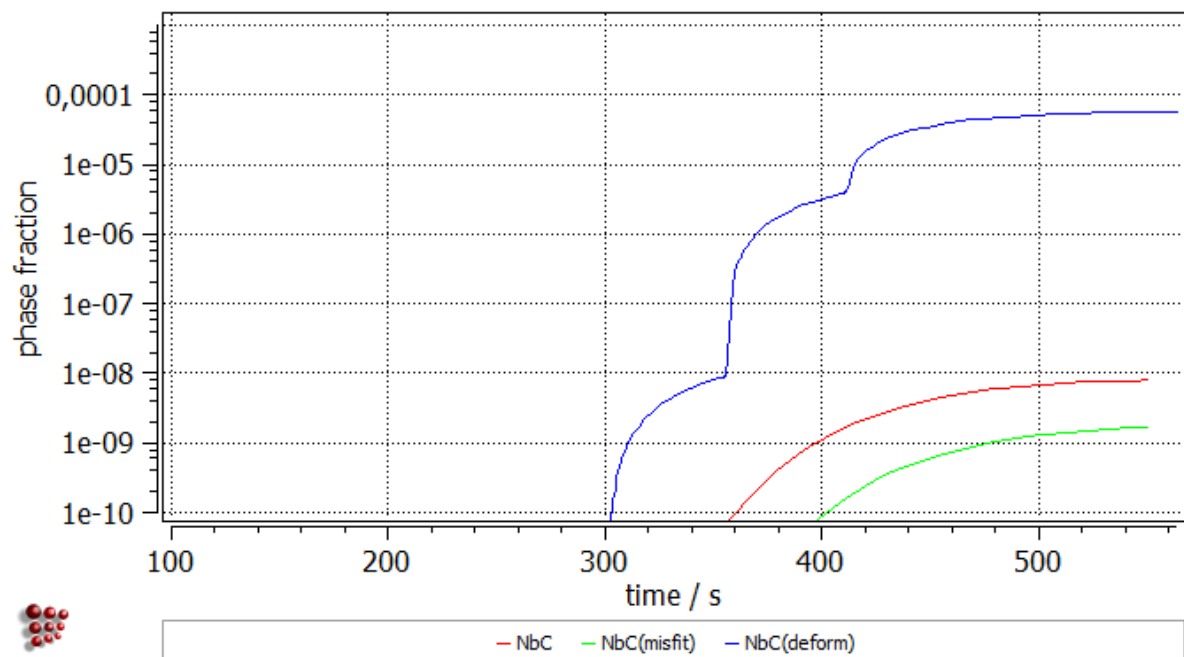
DEACTIVATION OF THE VOLUMETRIC MISFIT

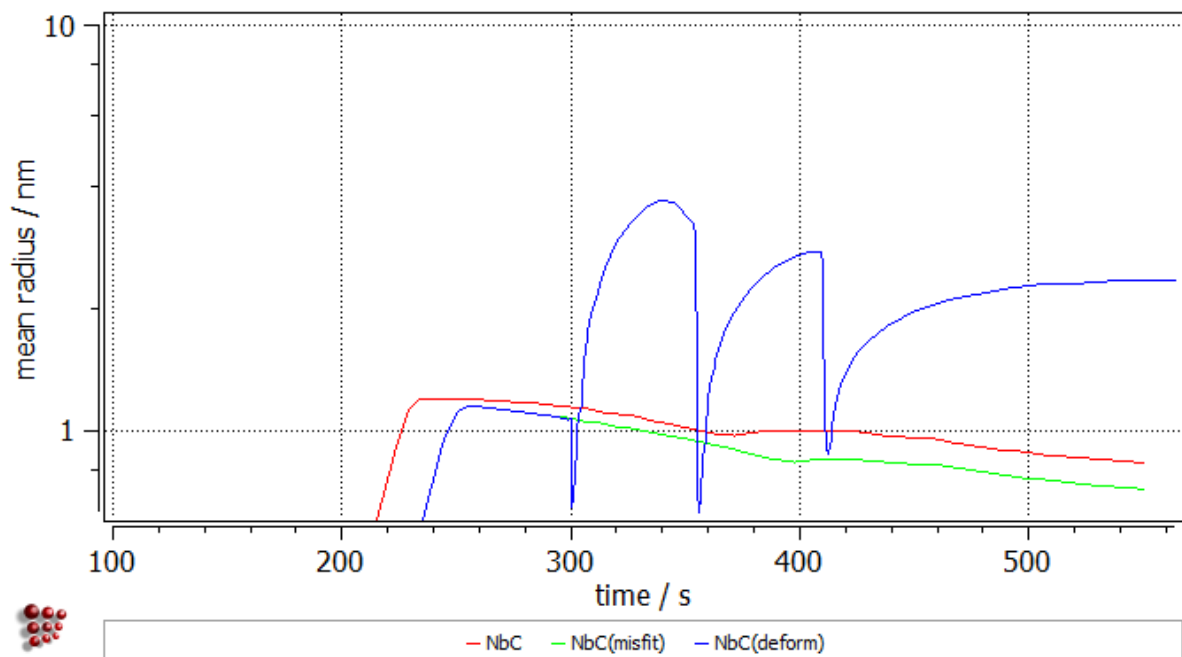
As previously mentioned, some volumetric misfit might be present related to the precipitates appearing in the grains, decreasing thus their nucleation rate. However, the stress introduced during the applied deformation can cancel this effect. To account for this in MatCalc, clicking on **'Global' → 'Phase status'** and select the **'Nucleation' → 'Controls'** tab. Put a checkmark at **'ignore misfit stress during deformation'** for both precipitate phases. Click on **'OK'** to close the window.



KINETIC SIMULATION

Click on '**Global**' → '**Buffers**' → '**Create**' to create a new buffer with the name '**Deformation**'. Afterwards, click on '**Calc**' → '**Precipitation kinetics**' and select the deformation treatment. Start the calculation by clicking on '**OK**'. The results of the precipitation kinetics calculation are shown now with the blue curve.





A considerable difference of three order of magnitudes is observed in the phase fraction of the precipitates. The same difference could be noticed for the number density. In both diagrams, three steps for the increase can be distinguished. The curve for the mean radius has a wavy form showing minima at the time frames of the sudden increases of the phase fraction and number density.

T22: RECRYSTALLIZATION ON SUBGRAIN BOUNDARIES

***This tutorial was tested on
MatCalc version 6.00 rel 0.282
license: free
database: mc_fe.tdb; mc_fe.ddb***

CONTENTS

- Activation of recrystallization model
- Kinetic simulation of recrystallization process

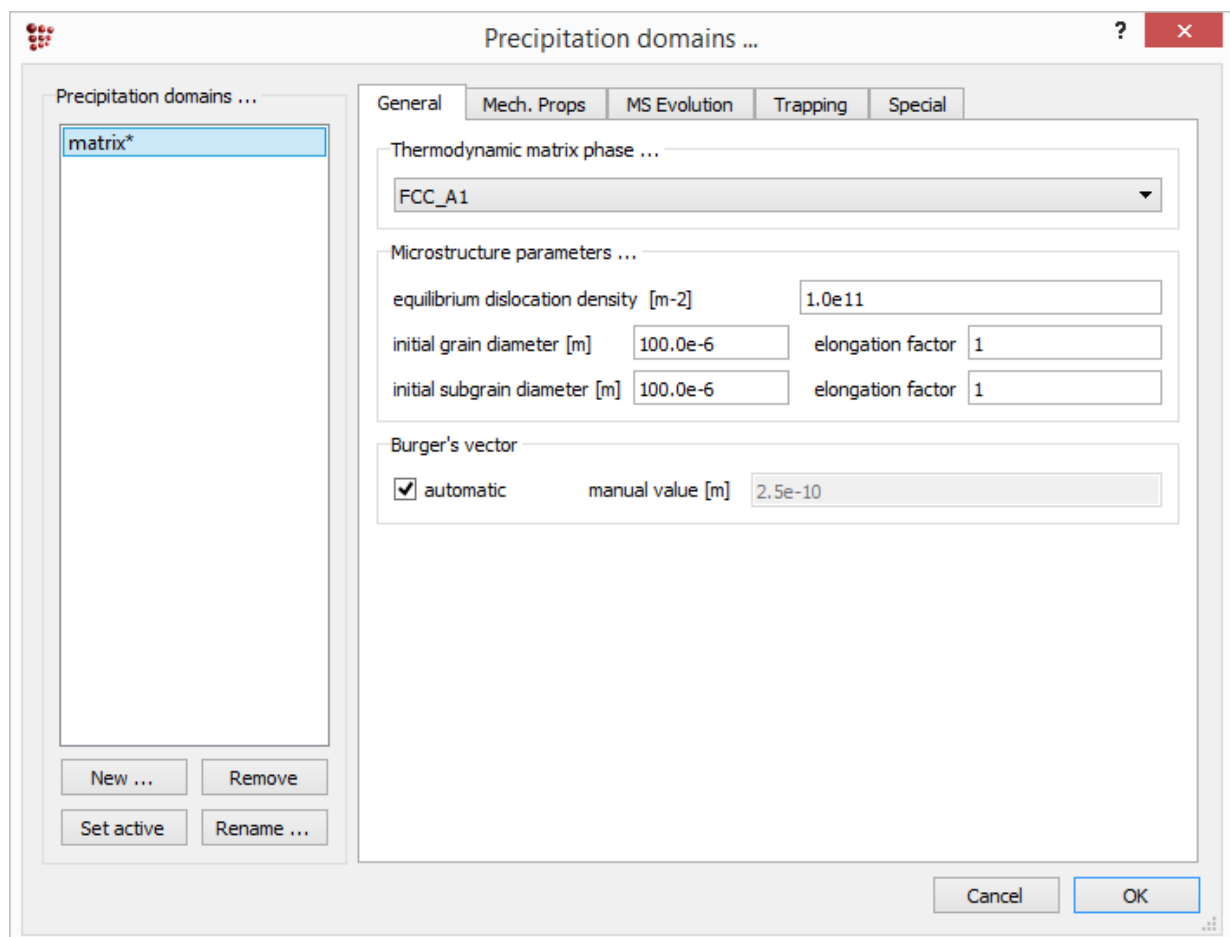
Deformation of the material introduces new dislocations into the microstructure. These surplus dislocations will create the substructure by ordering themselves into the subgrain walls during the recovery process. MatCalc includes a model describing the transformation of the newly subgrains into the new recrystallized grains, as described at Buken et al. This tutorial shows the procedure to activate the recrystallization model, presents the typical result of the recrystallization kinetics simulation and discusses the output values of the parameters obtained during the simulation.

SETTING UP THE SYSTEM

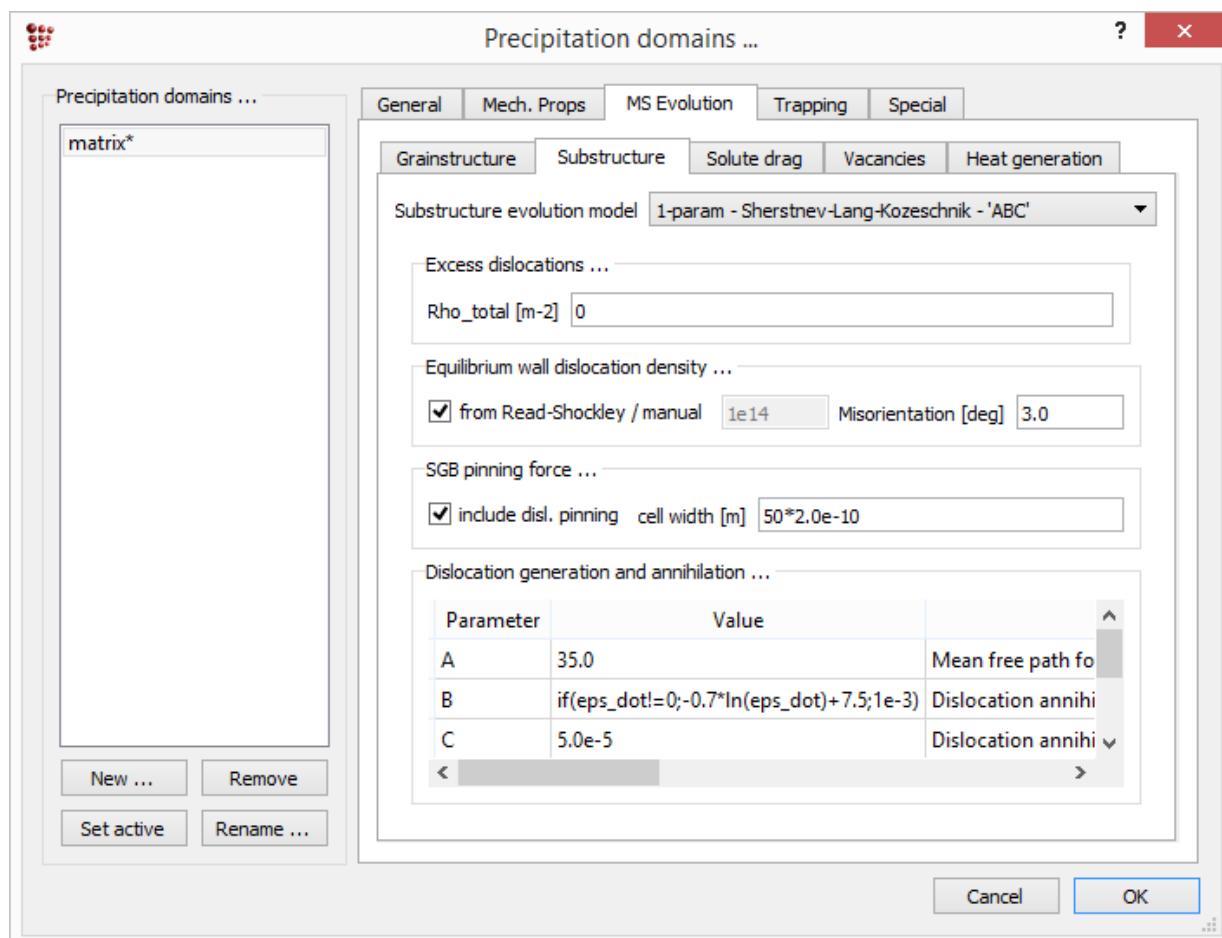
Create a new workspace and open the '**mc_fe.tdb**' database. Select the elements '**Fe**' and '**C**', together with the '**FCC_A1**' phase. Click on 'Read' instead of 'Read & Close', as the subsequent step is to read the diffusion database in this window. Select '**Diffusion data**' on the left side and read the '**mc_fe.ddb**' database. Enter the composition of **0.2 wt.% C**. Click on '**Set start values**' and calculate an initial equilibrium at 1200°C.

PRECIPITATION DOMAINS AND PHASES

Create a precipitation domain called '**matrix**' in the 'Precipitation domains ...' window. Select **FCC_A1** as the **thermodynamic matrix phase**.



In the current recrystallization model, the newly recrystallized grains form from subgrain created during the recovery process following the material deformation. First, the subgrain formation and size evolution will be investigated. The subgrains are generated by the ordering of the excess dislocations introduced during the deformation process. Hence, the next thing to do will be to activate the substructure evolution model. Switch to the '**MS Evolution**' tab, select '**Substructure**' tab inside and choose '**1-param - Sherstnev-Lang-Kozeschnik - 'ABC'**' as the model for the substructure evolution.



In this tutorial, the default model parameters will be used for the demonstration so click on **'OK'** to close this window.

THERMO-MECHANICAL TREATMENT

Now, define the thermo-mechanical treatment which will consist of the deformation segment and the subsequent annealing segment. For the sake of simplicity, the whole simulation will be performed at the constant temperature of 1200°C. In **'Global' → 'Thermo-mech. treatments ...'** create a new treatment with the name **'tmt'**. Next, create a segment in which the austenite domain will be deformed to the accumulated strain value of **'0,1'**. In **'MSEvolution'** tab, set the **'eps-dot'** (strain rate) value to **'1'**. Back in **'General'** tab, the **'Start temperature'** is to be set to **'1200°C'**.

Edit t/m treatment segment ...

General | **MS Evolution**

Temperature ...

Start temperature:

Ramp control ...

Accumulated Strain

End temperature:

Heat/Cooling Rate:

Delta-Time:

Accumulated strain:

Store Interval ...

Intervals: ☐ lin

log scale factor ☒ log

☐ reset store counter

Precipitation Domain ...

☐ inherit from previous segment

☒ select

Comment | **Pre-Segment Script** | **Post-Segment Script**

Edit t/m treatment segment ...

General | **MS Evolution**

deformation mode

eps-dot in

Options ...

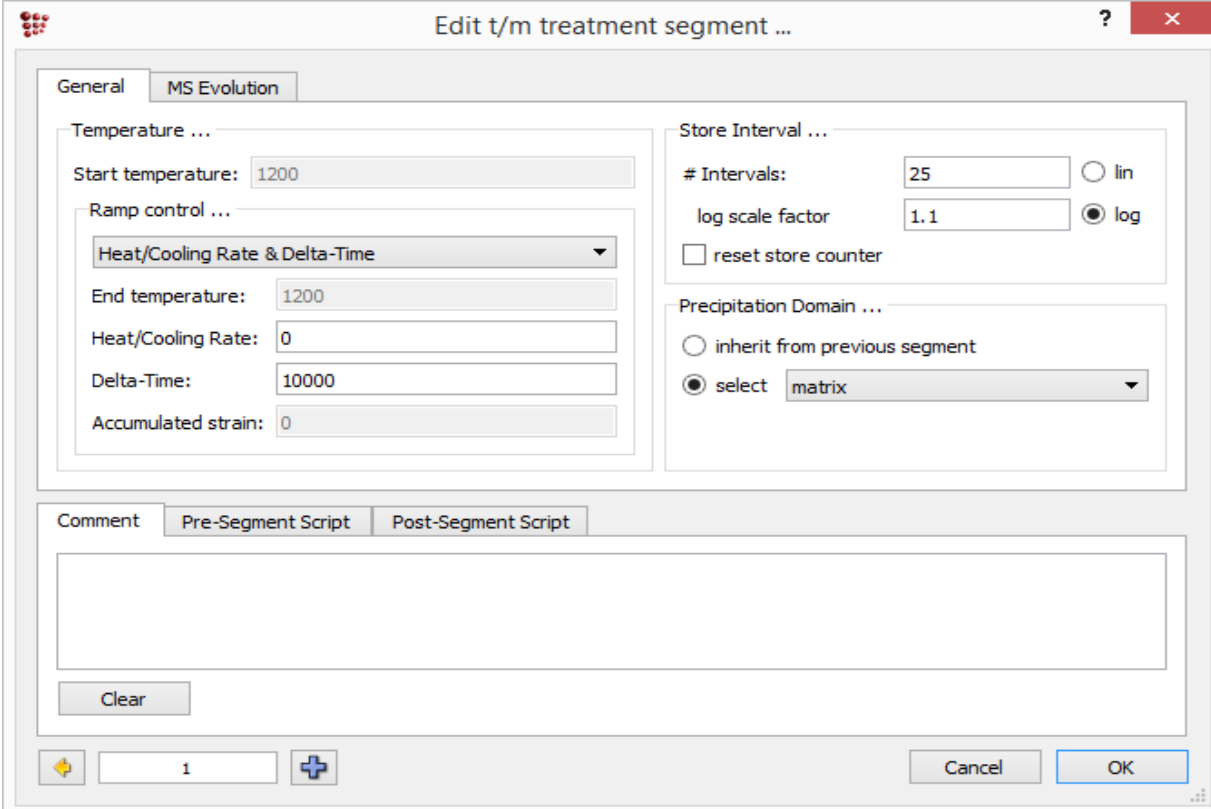
☐ reset excess vacancies ☐ break up particles

☐ reset X_recristallized ☐ release gb precipitates

☐ reset trap partitioning

Comment | **Pre-Segment Script** | **Post-Segment Script**

In the next segment, the material will be held isothermally at 1200°C. Select “Heat/Cooling Rate & Delta-Time” in “Ramp control” field and set the rate to '0' and the segment time to '10000' seconds.



Edit t/m treatment segment ...

General | MS Evolution

Temperature ...

Start temperature: 1200

Ramp control ...

Heat/Cooling Rate & Delta-Time

End temperature: 1200

Heat/Cooling Rate: 0

Delta-Time: 10000

Accumulated strain: 0

Store Interval ...

Intervals: 25 ☐ lin

log scale factor: 1.1 ☒ log

☐ reset store counter

Precipitation Domain ...

☐ inherit from previous segment

☒ select matrix

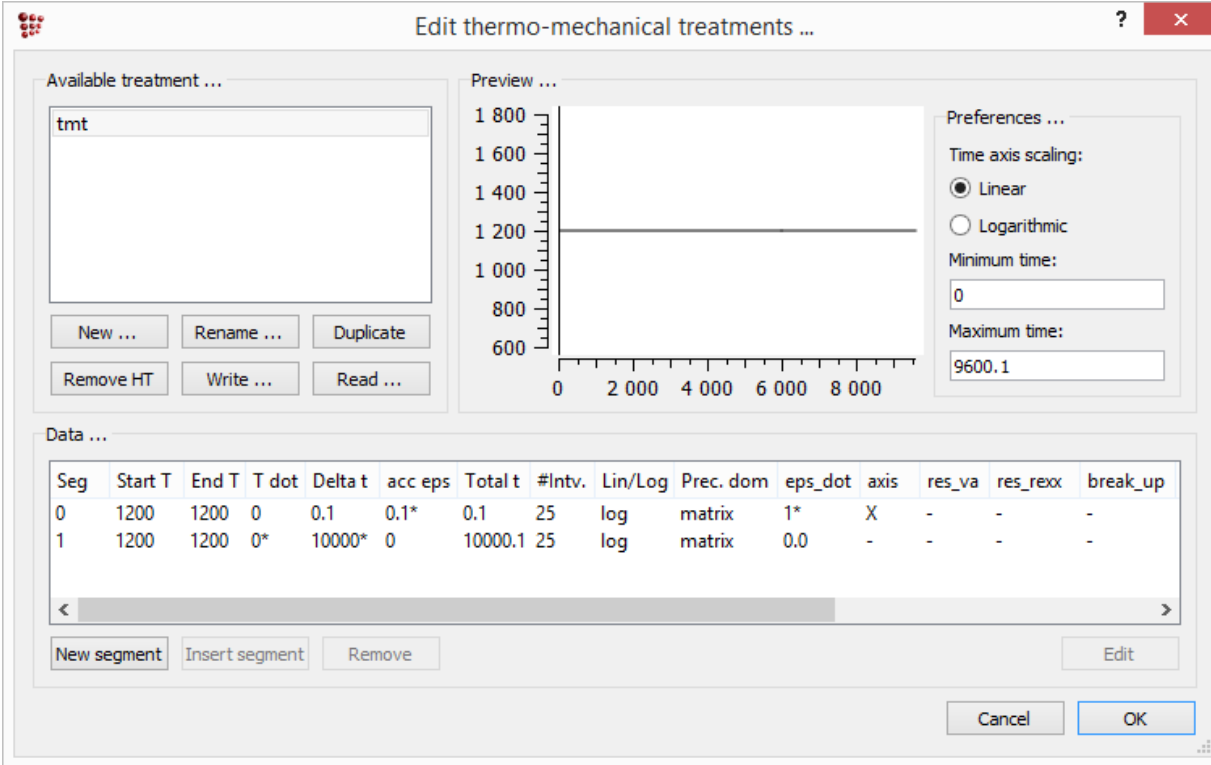
Comment | Pre-Segment Script | Post-Segment Script

Clear

1

Cancel OK

The settings for the whole treatment are summarized below.



Edit thermo-mechanical treatments ...

Available treatment ...

tmt

New ... Rename ... Duplicate

Remove HT Write ... Read ...

Preview ...

1 800

1 600

1 400

1 200

1 000

800

600

0 2 000 4 000 6 000 8 000

Preferences ...

Time axis scaling:

☒ Linear

☐ Logarithmic

Minimum time: 0

Maximum time: 9600.1

Data ...

Seg	Start T	End T	T dot	Delta t	acc eps	Total t	#Intv.	Lin/Log	Prec. dom	eps_dot	axis	res_va	res_rexx	break_up
0	1200	1200	0	0.1	0.1*	0.1	25	log	matrix	1*	X	-	-	-
1	1200	1200	0*	10000*	0	10000.1	25	log	matrix	0.0	-	-	-	-

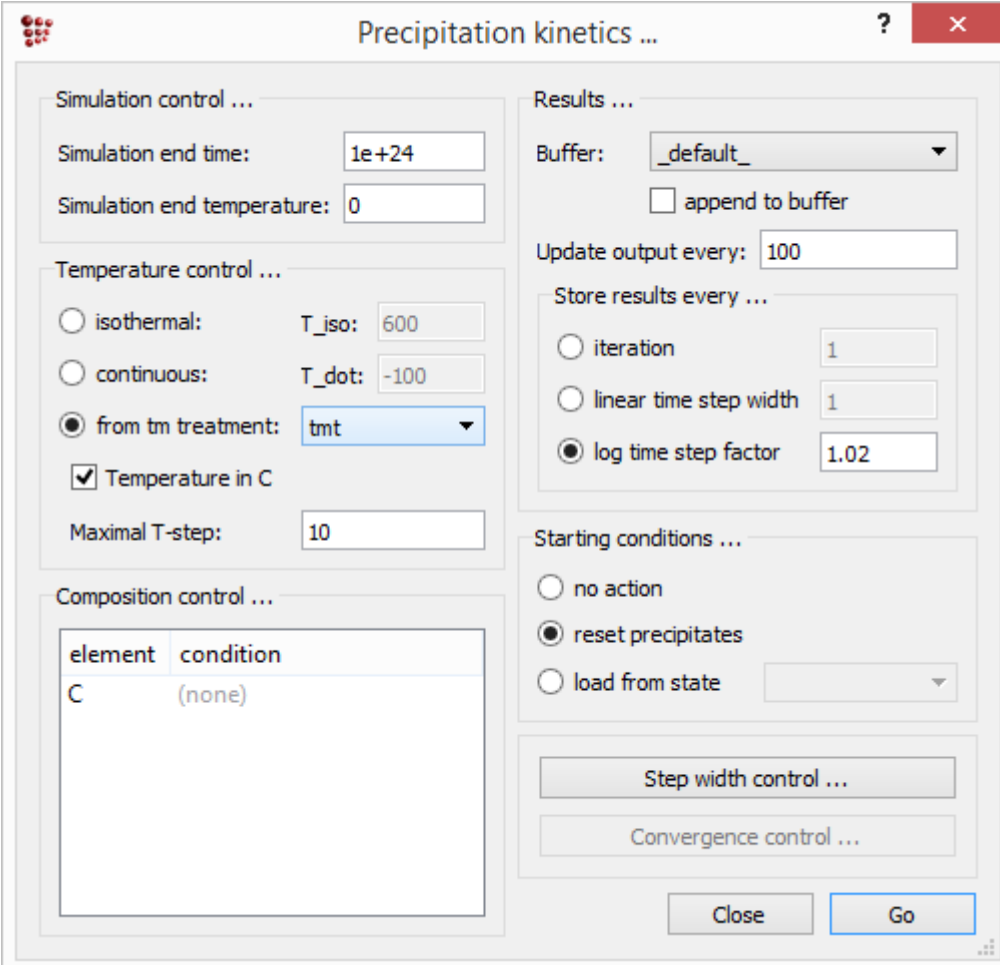
New segment Insert segment Remove Edit

Cancel OK

Close the editor window by clicking 'OK'.

KINETICS SIMULATION OF THE DEFORMATION PROCESS

With all the setup procedures done, perform the kinetics simulation. Click on 'Calc' → 'Precipitation kinetics'. Select the 'tmt' treatment in the 'Temperature control ...' area and click on 'Go'.



Precipitation kinetics ...

Simulation control ...

Simulation end time:

Simulation end temperature:

Temperature control ...

☐ isothermal: T_iso:
☐ continuous: T_dot:
☒ from tm treatment:
☒ Temperature in C
 Maximal T-step:

Composition control ...

element	condition
C	(none)

Results ...

Buffer:
☐ append to buffer

Update output every:

Store results every ...

☐ iteration
☐ linear time step width
☒ log time step factor

Starting conditions ...

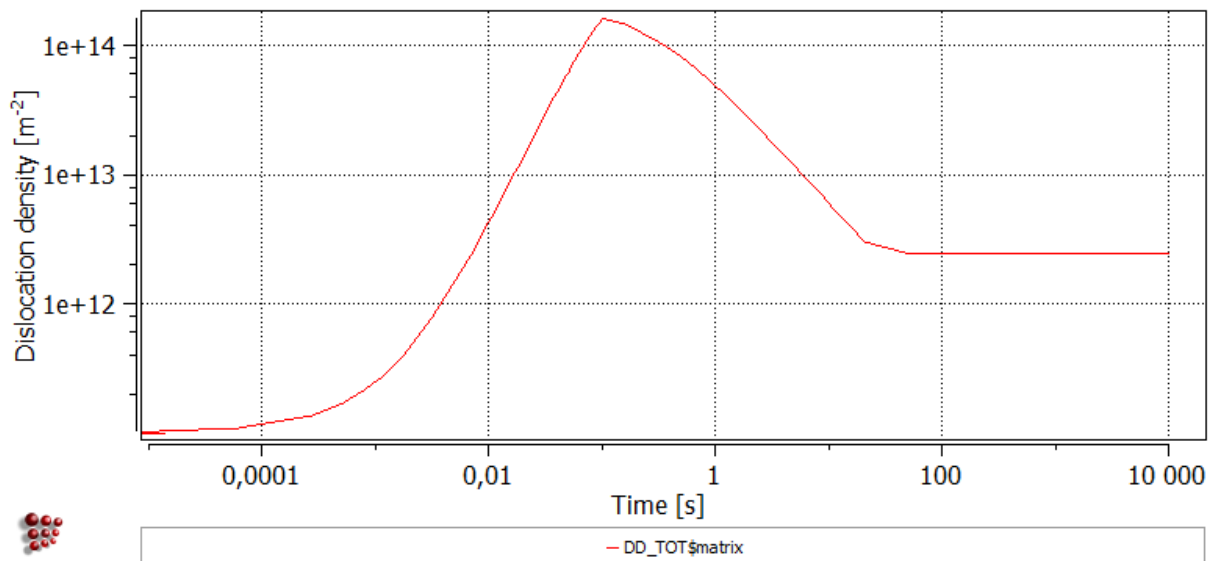
☐ no action
☒ reset precipitates
☐ load from state

Step width control ...

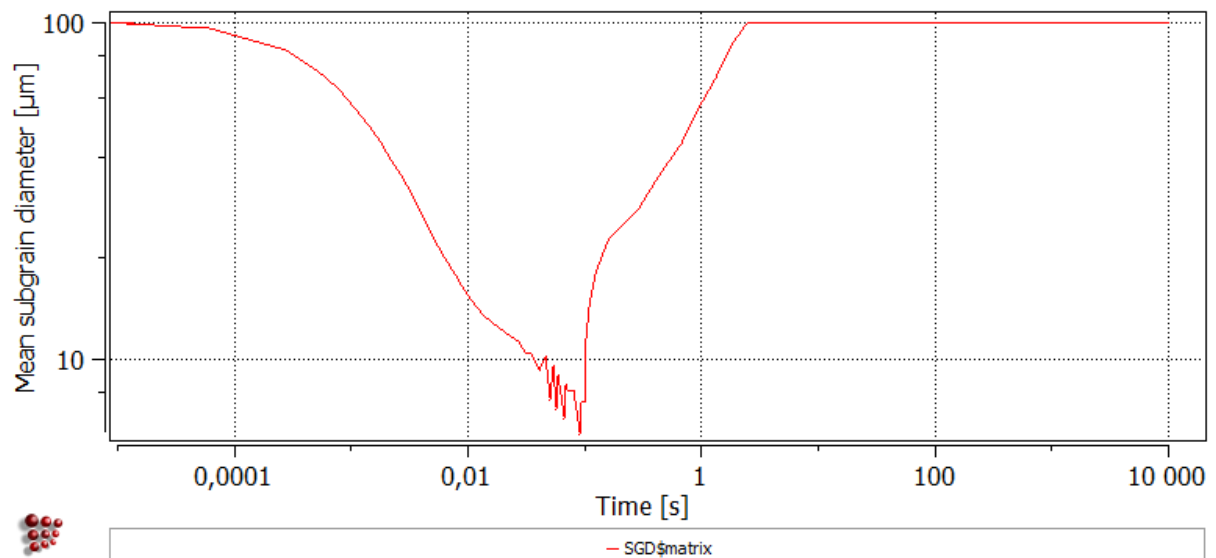
Convergence control ...

Close Go

Once the calculation is completed, create a plot visualizing the dislocation density. In menu 'View', click on 'Create new window...' and select '(p1) Plot core: XY-data' plot type. Drag and drop 'DD_TOT\$matrix' variable which is located in the 'prec_domain struct sc' group in 'variables' window. Set the x- and y-axis to logarithmic scale and start the x-axis scaling at 1e-5. Rename the x-axis to 'Time [s]' and the y-axis to 'Dislocation density [m⁻²]'. Switch on the major grids for both axes.



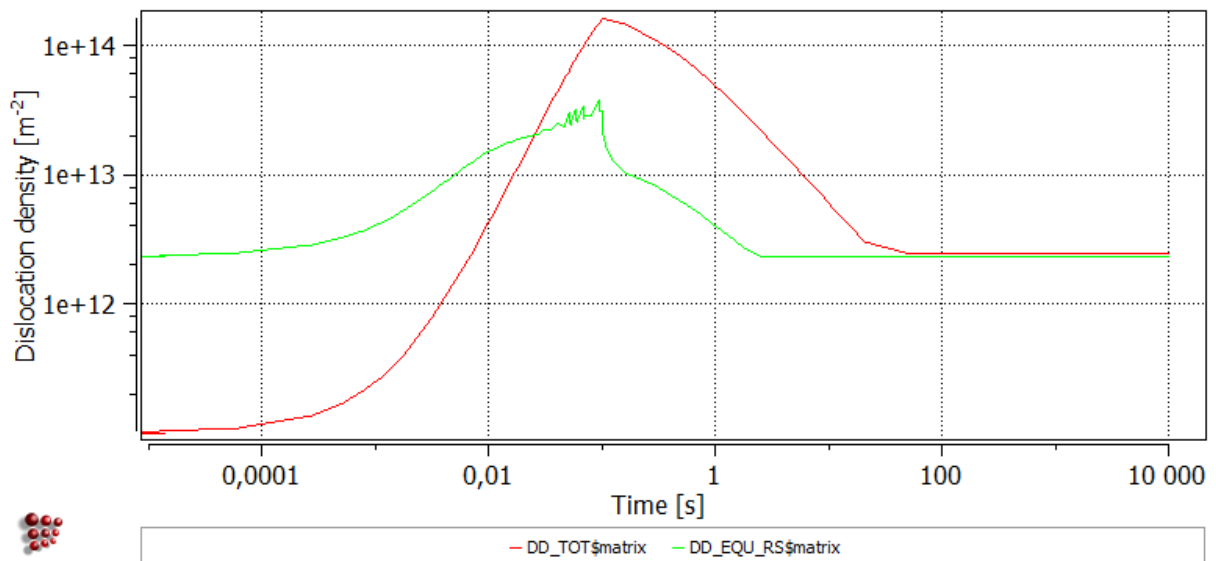
As might be expected, the plot shows an increase of the dislocation density during the deformation segment which lasts up to 0,1 second. Afterwards, the dislocation density falls down to approx. 2×10^{12} which corresponds to the recovery process during the subsequent isothermal holding at 1200°C . In order to investigate the effect on the size of the forming subgrains, create a new plot depicting the '**SGD\$matrix**' variable which represents the subgrain diameter. '**SGD\$matrix**' variable can be also found in the '**prec_domain struct sc**' group.



The subgrain diameters drops initially from about 100 micrometers down to about 7 micrometers at 0,1 seconds. Afterwards, it rises again reaching the initial value. The stage of subgrain decrease is not to be interpreted directly, as the subgrains are formed during recovery rather than during deformation stage. It is a consequence of the MatCalc setting which sets the initial value of subgrain diameter equal to the initial value of the grain diameter. Then, the subgrain size is calculated inversely to the square root of the dislocation density, in accordance

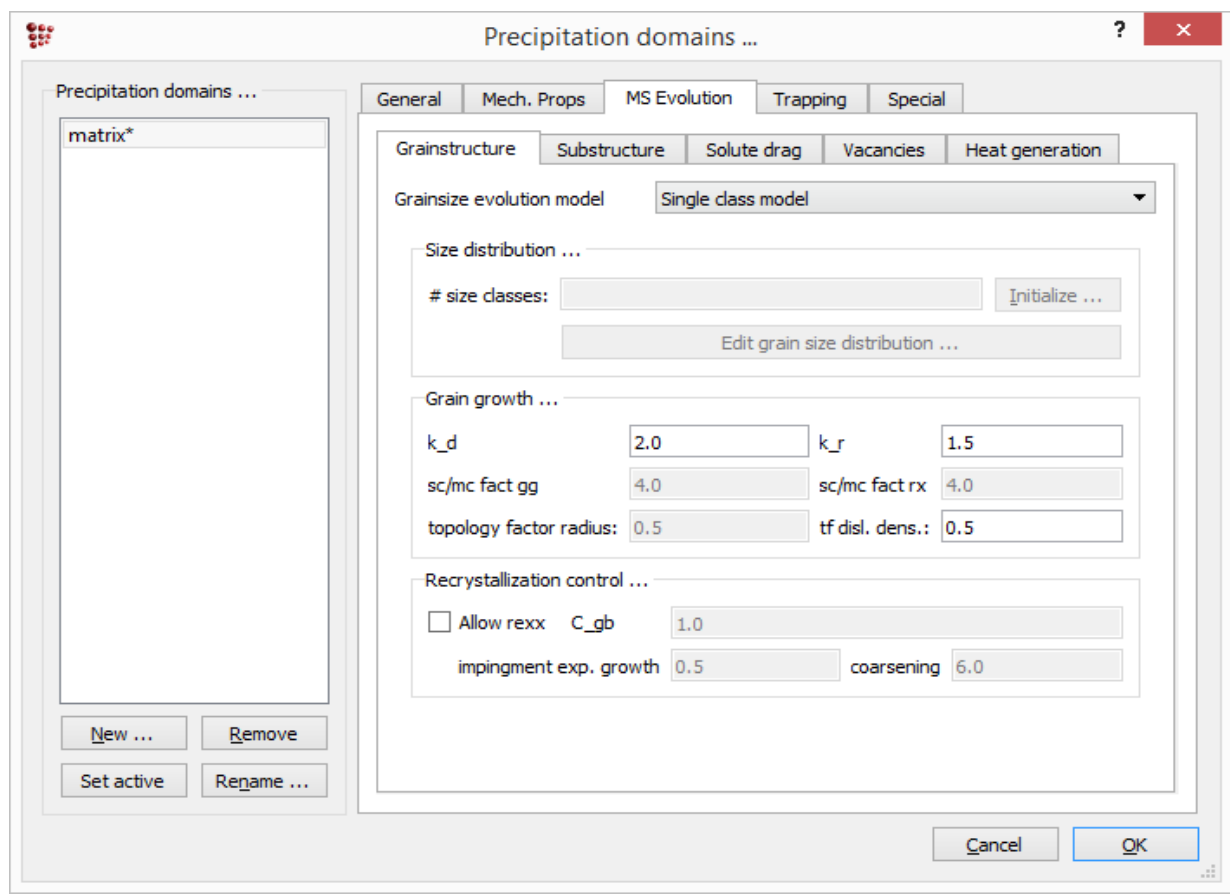
with the similitude principle. As the recovery process starts, it is assumed that the subgrains are immediately formed with the predicted size of 7 micrometers. These subgrains grow afterwards in a similar way as the grains would do - there is a model which correlates the growth rate with the inverse of the subgrain diameter. During the recovery step, the rising subgrain size corresponds to the falling dislocation density. After almost 3 seconds, the subgrain size reaches the initial value of 100 micrometers and cannot grow further as the limiting grain size remains at this value. The dislocation density decreases further down to about $2 \cdot 10^{12} \text{ m}^{-2}$. After reaching this value at about 35 seconds, it remains steady till the end of the simulation.

One might ask, why the dislocation density remains at this value rather than decreasing further to the initial value of 10^{11} m^{-2} . This happens as MatCalc proceeds with the dislocation annihilation till the equilibrium wall dislocation density value is reached, as defined in the substructure model setting. The last simulation was performed on the default setting which sets this value to the one required for the presence of the subgrains with the given size, as proposed by Read and Shockley. In the last case, the subgrains could not grow beyond 100 micrometers. It was already mentioned before, that the subgrain size is calculated from the dislocation density on the basis of the similitude principle which relates these two parameters. In the same manner, it is possible to calculate dislocation density which are geometrically needed for the given subgrain size and the given misorientation angle between the neighboring subgrains. As might be recalled from the substructure model settings, the misorientation angle of 3 degrees was used in the last calculation. The limiting value of the dislocation density coming from the discussed geometrical constraint is represented by the variable '**DD_EQU_RS\$austenite**'. Drag and drop this variable on the dislocation density plot. The first observation is that the initial value for the limiting density is above the simulated actual density value. As mentioned above, this stage is not to be directly interpreted, as the subgrains are not forming during the deformation yet. During the recovery period, the limit value proceeds according to the subgrain size and reaches a plateau at about 3 seconds, when the subgrains do not grow anymore. The limit density curve is joined by the actual density one at about 35 seconds, after which nothing more happens in the system.



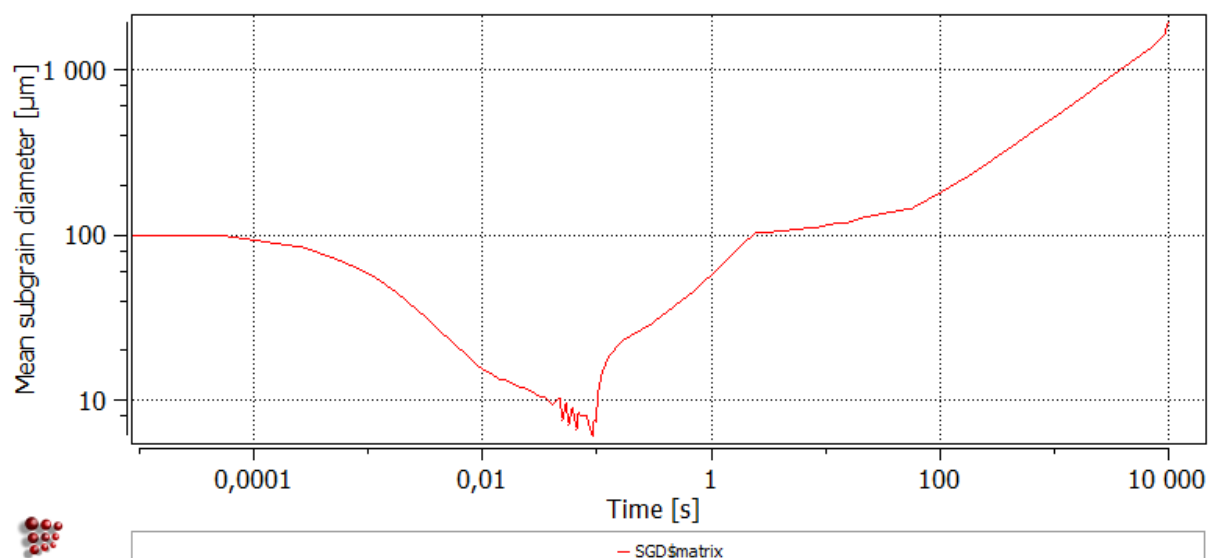
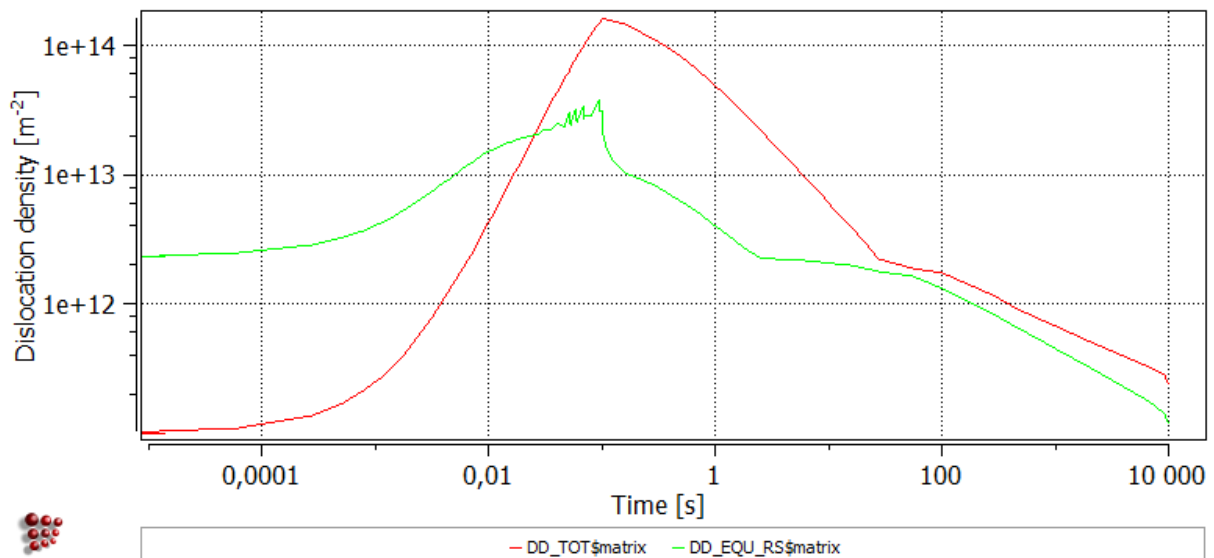
INTRODUCING GRAIN GROWTH

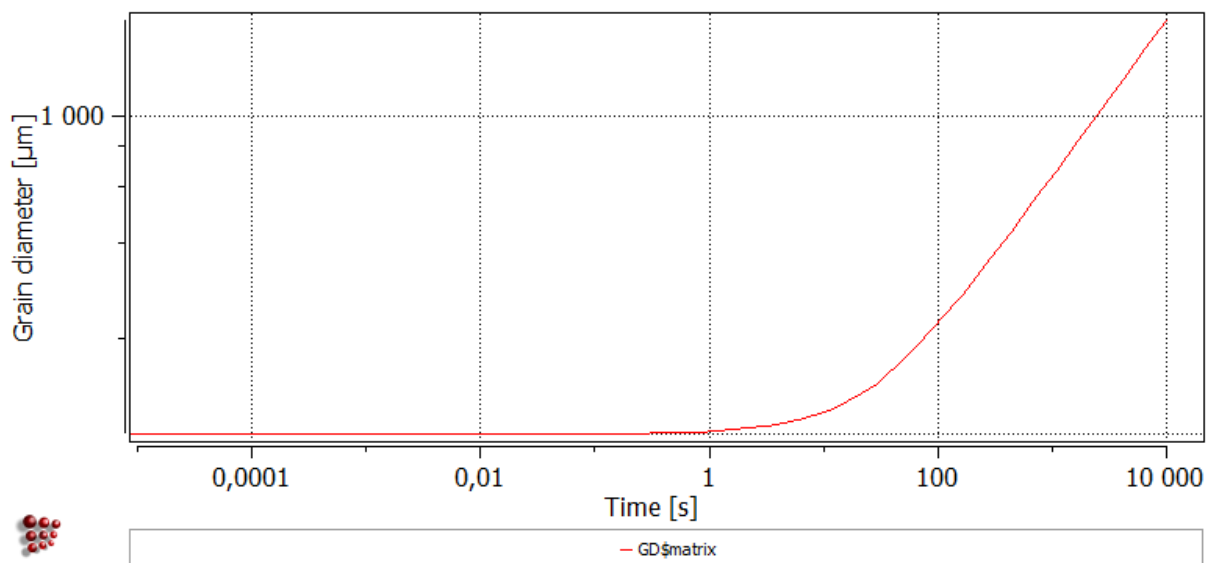
In the next simulation, the grain growth model will be activated, so that the constraint on the subgrain growth will be removed. In 'Precipitation domains' window, select the **'MS Evolution tab'** and click on **'Grainstructure'** tab there. In the field **'Grainsize evolution model'** select **'Single class model'**. Leave all parameters on default value.



By clicking on 'Global' → 'Buffers' → 'Rename', rename the current buffer to 'deformation_only'. Next, in 'Global' → 'Buffers' click on 'Create' and name the new buffer as 'deformation&growth'. Create a new plot showing the grain diameter. Rename the y-axis to 'Grain diameter [μm]', set the factor to '1e6' and switch the y-axis to logarithmic type. Drag and drop the variable 'GD\$matrix' on the plot. At the moment, only a straight line is visible, as the grain growth was kept constant in the last simulation. Right click on the plot and click on 'Duplicate and lock all series'. Afterwards, repeat the calculation by clicking on 'Calc' → 'Precipitation kinetics...' and clicking 'OK' in the appearing window.

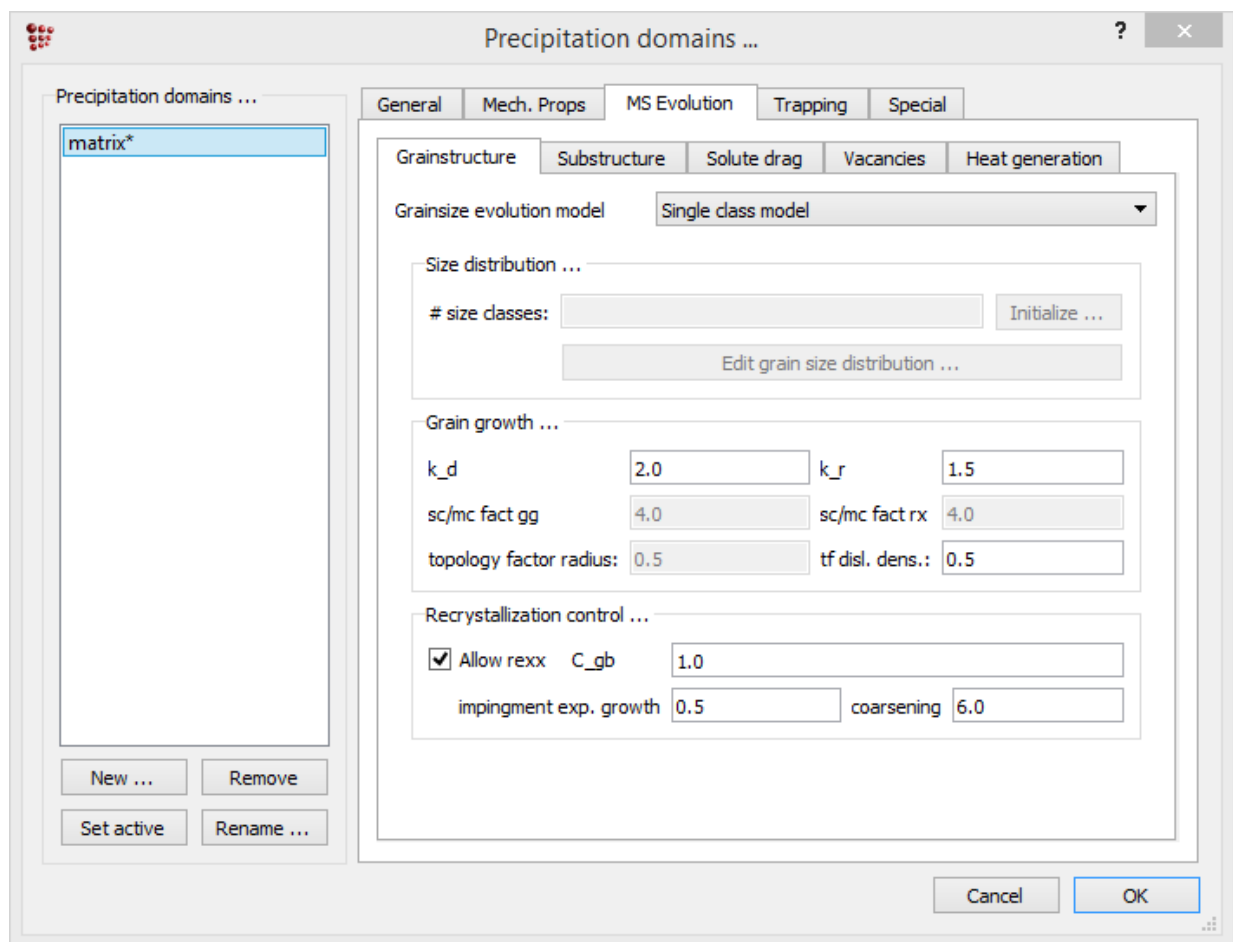
After the calculation is done, switch the buffer relevant to the plots to the current one. In the 'options' window, select 'deformation&growth' in the 'core buffer' field. One can immediately notice the difference in the curves at the recovery stage. Increasing grain diameter allows for the further growth of the subgrains. This results in the further decrease of the dislocation density.





INTRODUCING RECRYSTALLIZATION

It is time to activate the recrystallization model. In 'Precipitation domain' window, select again the '**MS Evolution**' and '**Grainstructure**' tab there. In the '**Recrystallization control...**' section put a checkmark in '**Allow rexx**' field.



In 'Global' → 'Buffers' click on 'Create' and create a new buffer named 'Recrystallization'. Next, create three more plots in the plot window. Use the following y-axis settings for the plots:

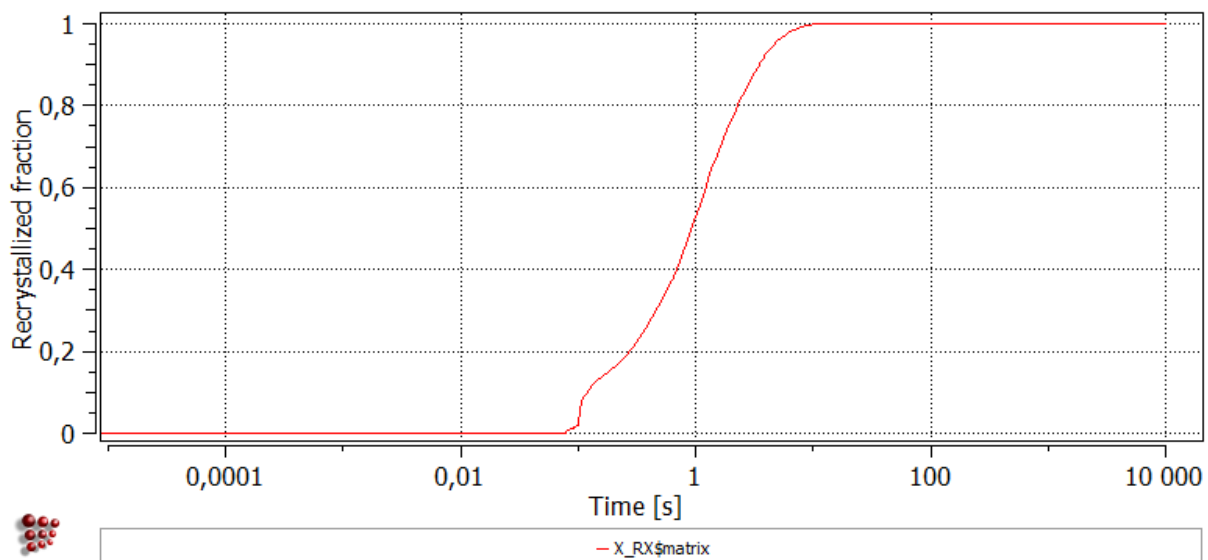
- **Title:** Nucl. rate of rex. grains [$\text{m}^{-3}\text{s}^{-1}$], **type:** log
- **Title:** Number density of grains [m^{-3}], **type:** log
- **Title:** Recrystallized fraction

Drag and drop the following series on the plot:

- 'RX_NUCL_RATE\$matrix' (can be found in 'prec_domain ms evolution' variables group)
- 'NG\$matrix', 'NG_DEF\$matrix', 'NG_RX\$matrix' (can be found in 'prec_domain struct sc' variables group)
- 'X_RX\$matrix' (can be found in 'prec_domain struct sc' variables group)

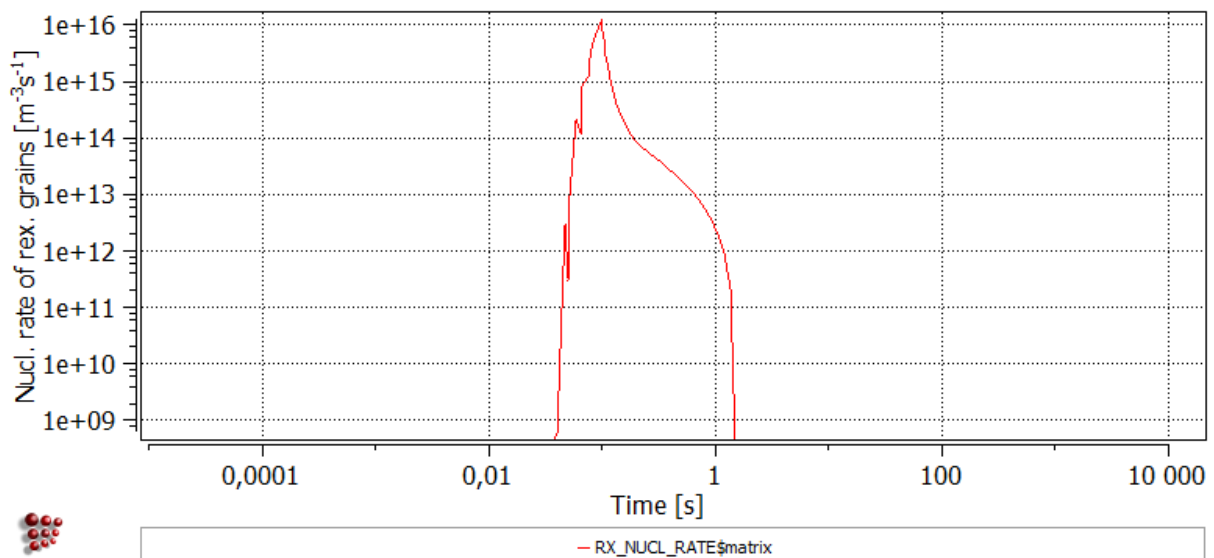
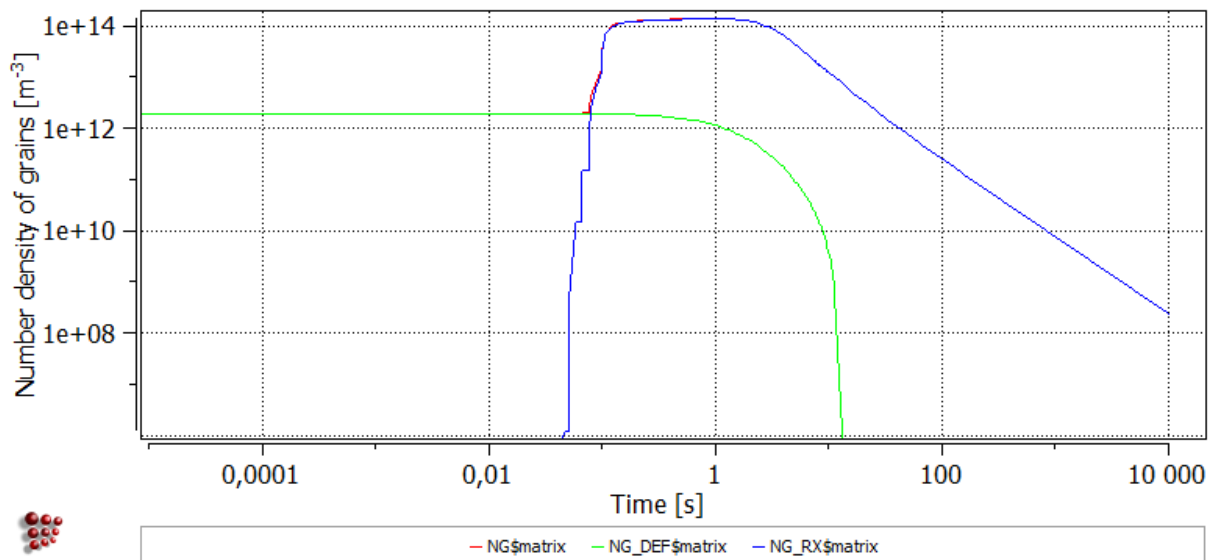
Additionally, add the series 'GD_DEF\$matrix' and 'GD_RX\$matrix' to the plot of grain diameters.

With all these plots present, perform once again a kinetic simulation. Once it is completed, a picture of the recrystallization progress in the system is available. Looking at the last plot of recrystallized fraction for the matrix, one can notice that the structure is fully recrystallized. The process seems to happen between the 0,1 and 10 seconds.



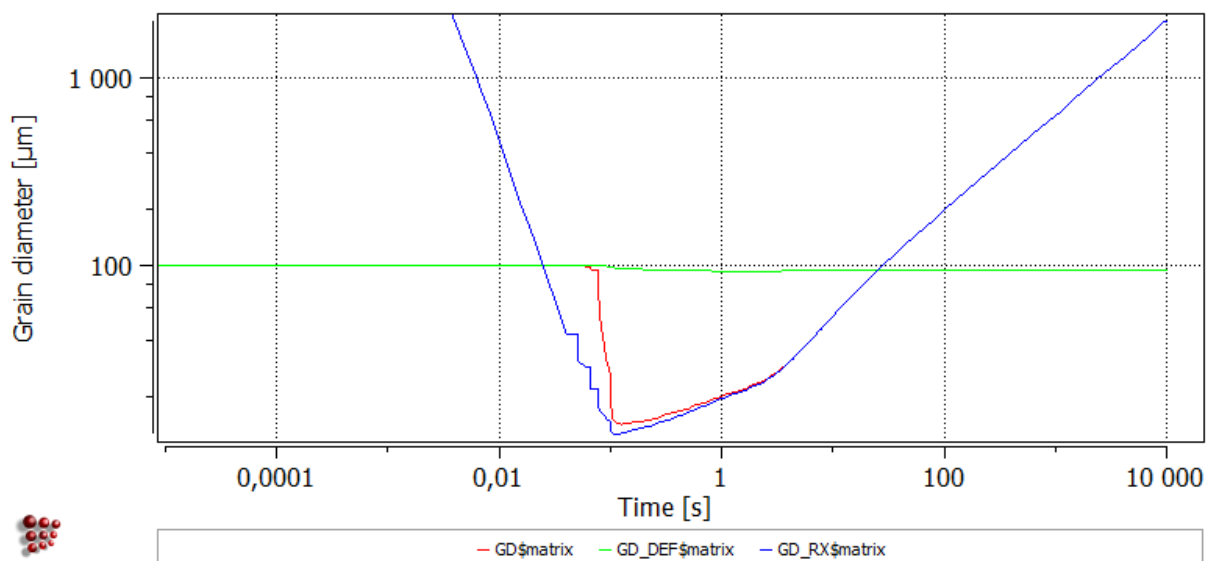
Looking on diagram showing the grain number densities, one can notice that the “old” microstructure of the deformed grains, represented with the variable 'NG_DEF\$matrix', with the initial density of slightly above $1\text{e}12 \text{ m}^{-3}$ decreases gradually and vanishes at the end of the recrystallization process. The curve representing the number of the recrystallized grains (variable 'NG_RX\$matrix') appears already before 0,1 seconds and grows fast, showing a maximum value at about $1\text{e}14 \text{ m}^{-3}$ and then continues to decrease to the end of the simulation.

This analysis is supported by the plot of nucleation rates of recrystallized grains, which shows that the nucleation phase for the recrystallized grains starts around the time of 0,05 seconds and lasts to about 1,5 seconds. The end of the nucleation phase coincides obviously with the maximum observed for the number density of the recrystallized grains. The total number density of grains, represented by the variable 'NG\$matrix' is just a superposition of the two previous values.

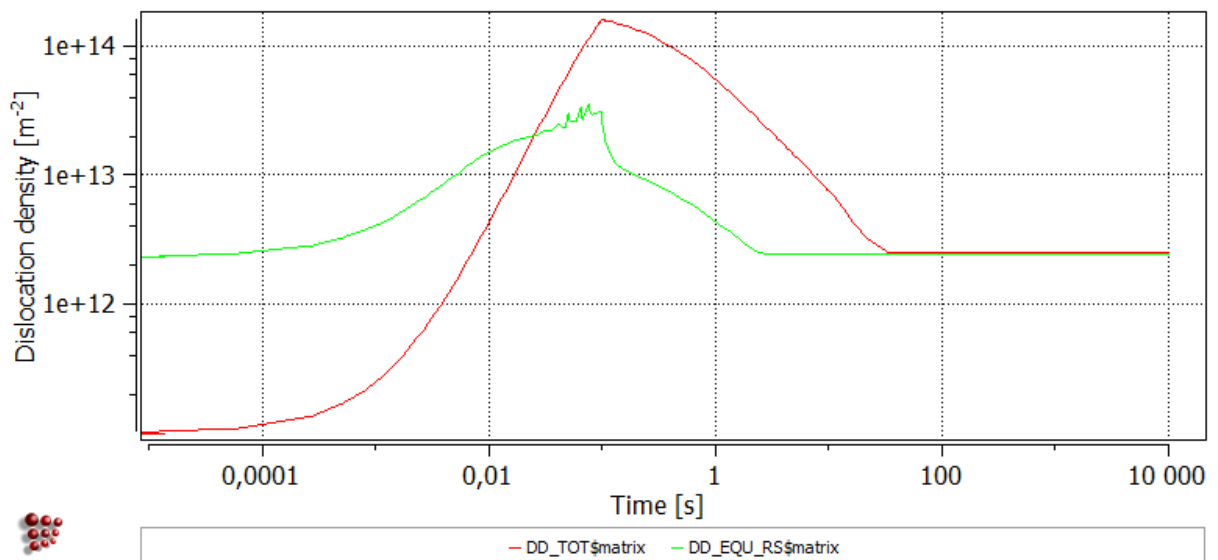
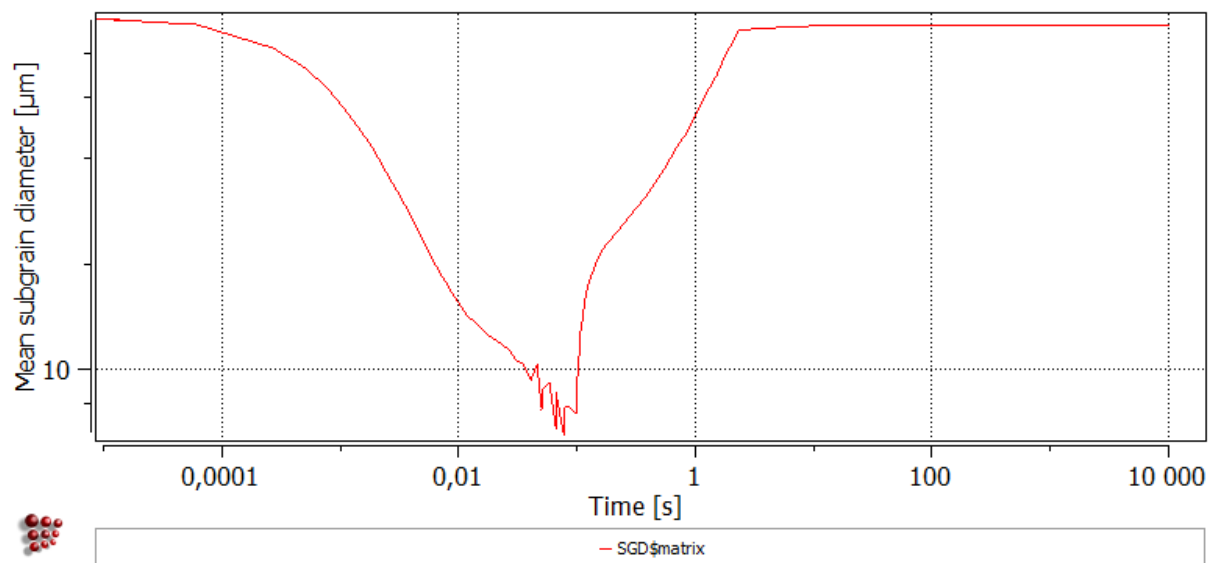


The plot representing the grain diameter (with y-axis scaling limited to 2000 micrometers) gives some further information. The curve 'GD_DEF\$matrix' representing the size of the deformed ("old") grains initializes at 100 micrometers. The curve 'GD_RX\$matrix' representing the size of the recrystallized ("new") grains initializes at some high value and decreases down to about 13 micrometers. Obviously, a physical interpretation for the recrystallized grain size is reasonable only for the process time when such grains are present at all, i.e. once the number density of recrystallized grains gets a positive value. The mean value for the grain diameter

observed in the microstructure ('GD\$matrix' curve) decreases gradually from the deformed value towards the recrystallized value. Growth process of the recrystallized grain can be observed after the deformation process ends. On the contrary, the diameter of the deformed grain decreases a little, as these grains are “consumed” by the newly formed structure. Of course, there is again no interpretation possible for the deformed grain size for the simulation time with zero number density of these grains. Once the microstructure is fully recrystallized, a grain growth is observed. This coincides with the reduction of the nucleation density representing an occurrence of the grain impingement.



Interestingly, the results for the subgrain size and dislocation density are similar to the ones obtained in the simulation without grain growth. The subgrain size seems to be limited again short below 100 micrometers and the dislocation density remains steady at the according value. To interpret this outcome correctly, one needs to keep in mind that the subgrains are assumed to exist only in the deformed grains in the applied single class model. The first consequence of this fact is that the interpretation of the calculated subgrain size is relevant only for the time periods when the deformed grain is present in the system, i.e. till the microstructure is fully recrystallized. The other consequence is the limitation of the subgrain size which cannot get a value greater than the size of the deformed grain. As the deformed grain size did decrease during the simulation, the subgrain size growth also stops around 95 micrometers. The dislocation density remained also at the value corresponding to the simulated subgrain diameter.



T23: INTRODUCTION TO CELL SIMULATIONS: LONG-RANGE DIFFUSION

***This tutorial was tested on
MatCalc version 6.00 rel 1.000
license: free
database: mc_fe.tdb; mc_fe.ddb***

CONTENTS

- setting up a simulation grid
- assigning properties to cells
- setting up display of cell simulation results
- setting up simulation parameters
- boundary conditions

MatCalc can be used to carry out simulations of long-range diffusion problems, and problems in which diffusion is coupled with precipitation, using a finite-element method with the system divided into a number of cells. Many examples of the application of this functionality, in different systems and with different boundary conditions, can be found in the relevant part of the 'Examples' section. The present tutorial demonstrates a simple case for which an analytical solution of Fick's 2nd Law is available. The numerical and analytical solutions are compared.

The functionality for setting up and running diffusion simulations is only available through the scripting language and not through the GUI. This tutorial therefore also serves as a refresher for some of the basic scripting commands that we have already encountered, as well as introducing the new commands needed to set up and run diffusion simulations.

DESCRIPTION OF THE PROBLEM

Fick's Second Law of Diffusion is a partial differential equation of the form:

$$\left(\frac{\partial C}{\partial t}\right) = D \cdot \left(\frac{\partial^2 C}{\partial x^2}\right)$$

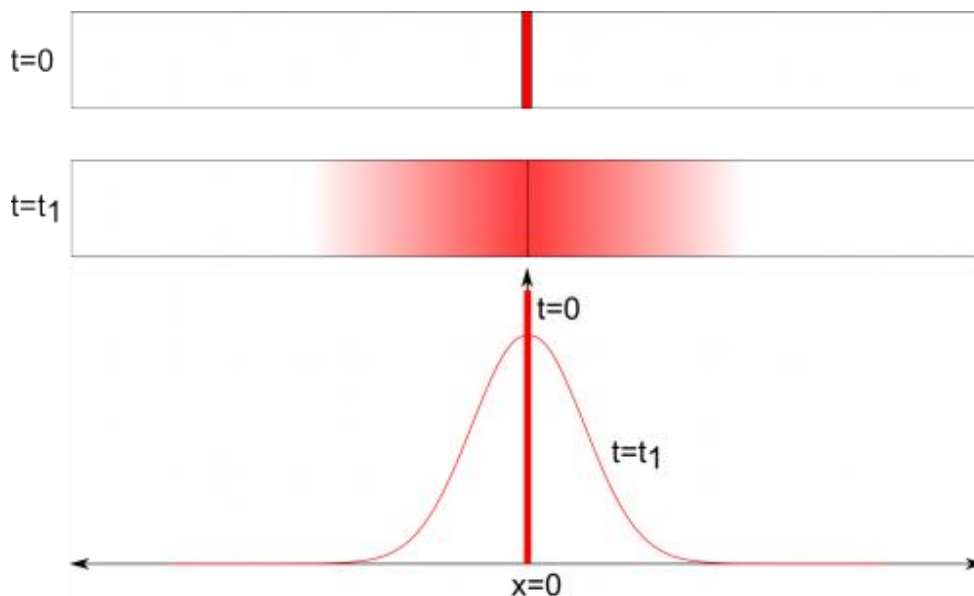
where D is the diffusion coefficient, which is here assumed to be independent of concentration. This equation can be solved to give the concentration C of the diffusing species as a function of distance x and time t . The form of the solution depends on the boundary conditions. In most cases, a numerical solution using finite-difference or finite-element methods is required, but there are some special cases in which an analytical solution is also available.

One of these is the thin-film solution, in which an very thin layer containing a finite amount of the diffusing species is sandwiched between two semi-infinite bars of material. The boundary conditions are that:

- initially, the concentration of the solute in the bar is zero; this is expressed mathematically as $C\{x=0, t=0\}=0$, where x is the distance from the midpoint marked by the central black vertical line in the diagram below, and
- the total amount of solute is finite and constant throughout the time period considered; this is expressed mathematically as

$$\int_{-\infty}^{\infty} C\{x, t\} dx = B,$$

where B represents the amount of solute in the system.



The standard solution when the boundary conditions are of this type is of Gaussian form:

$$C\{x,t\} = \frac{B}{2\sqrt{\pi Dt}} \cdot \exp\left(\frac{-x^2}{4Dt}\right)$$

In this tutorial, we will set up a cell-based numerical simulation of a situation that fulfils these conditions to a reasonably good approximation, i.e. a thin layer of FCC iron with a relatively high carbon content sandwiched between two bars of FCC iron with a very low carbon content. The results of this simulation will be compared with those obtained using the analytical solution.

SETTING UP THE SYSTEM

Start MatCalc and create a new script file as explained in Tutorial 13.

THERMODYNAMIC AND KINETIC SETUP

The first task that the script must perform is to create a new MatCalc workspace. Type the following command into your script window:

```
use-module core
```

This tells MatCalc to use the **core module**, which it selects at the beginning by default anyway; later in this tutorial we will see the use of the **simulation module**.

```
new-workspace
```

This creates a new workspace. If an existing unsaved workspace is open when the script is run, you will be prompted to save it. To disable this prompt, append `f` to the `new-workspace` command.

Some workspace information can be added as shown:

```
@$*****
$ enter workspace info
@$*****
@ set-workspace-info Script T23
@ set-workspace-info +Simulation of long-range diffusion of C
@ set-workspace-info +out of thin film
```

```
@ set-workspace-info +with matrix phase FCC_A1.
```

The next step is to set up the thermodynamic and kinetic data. Enter the following commands into your script window and save the script.

```
open-thermodyn-database mc_fe.tdb  
  
select-elements fe c  
  
select-phases FCC_A1  
  
read-thermodyn-database  
  
read-mobility-database mc_fe.ddb
```

Following this, define the variables that will specify the initial carbon content in the bar (`c_comp_bar_wp`) and the thin layer (`c_comp_layer_wp`) so that these can be used later. Note that the carbon content of the bar is set to be very low, but for numerical reasons it is not advisable to set this to exactly zero.

```
set-variable-value c_comp_bar_wp 1e-10  
  
set-variable-value c_comp_layer_wp 0.8
```

In the cell simulation, compositions must be entered in molar notation `un$c`. The code below enables you to enter a composition in weight percent (`wp`) and then save the composition in mole fraction as a variable for use in the cell simulation.

```
enter-composition wp c=c_comp_bar_wp  
  
set-variable-value c_comp_bar un$c  
  
enter-composition wp c=c_comp_layer_wp  
  
set-variable-value c_comp_layer un$c
```

Then set a temperature and calculate an equilibrium to initialise the system and check that everything is working OK.

```
set-temperature-celsius 1000  
  
calculate-equilibrium
```

At this stage, also specify the simulation time (in seconds) for subsequent use:

```
set-variable-value sim_time 1e7
```

Save the script. It is recommended to test it out at this stage to catch any typing errors before going further.

PRECIPITATION DOMAIN SETUP

Before setting up the cell simulation, you must define a **precipitation domain**, i.e. a matrix of phase FCC_A1; this is necessary for subsequent use in the cell simulation.

```
create-precipitation-domain aus_domain  
set-precipitation-parameter aus_domain X FCC_A1
```

CREATING THE SIMULATION GRID

The next step is to set up the cell simulation. First change to the **simulation** module:

```
use-module simulation
```

Define a variable representing the number of cells:

```
set-variable-value num_cells_x 99
```

Then create a simulation grid using the command:

```
create-simulation-grid num_cells_x 1 1
```

The three numbers here represent the number of cells in the x-, y- and z-directions, respectively. Define a variable representing the length of the bar:

```
set-variable-value barlength 0.099
```

Specify the dimensions in these directions (in m) using the command:

```
set-grid-coordinates barlength 1 1
```

and the geometry of the grid, using the command:

```
set-grid-geometry p
```

The three geometry options are:

- p - planar

- c - cylindrical
- s - spherical

To visualise this grid, create a new window of the type g5 (Paint grid: 2D cells):

```
new-gui-window g5
```

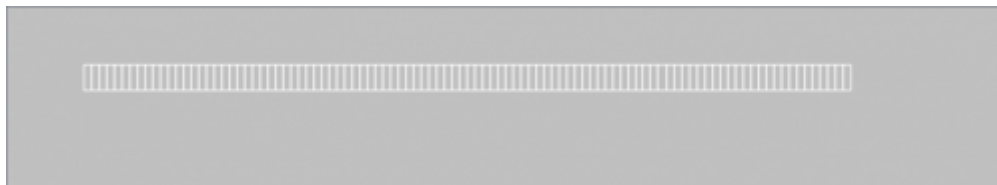
Give this window a name so that it can be referred to easily later. The variable `active_frame_id` used here is one of MatCalc's internal variables; see the section of the Reference book on internal variables for details.

```
set-variable-value paint_window_id active_frame_id
```

Modify the position, size and zoom level using the following two commands:

```
move-gui-window paint_window_id 0 100 750 160 $ change position and size
set-gui-window-property paint_window_id i Z 200 $ zoom 200%
```

The grid should now look as shown:



In the next section, properties will be assigned to the cells in the grid.

ASSIGNING PROPERTIES TO THE CELLS

For the diffusion simulation, it is necessary to create a **material** and assign to this the **precipitation domain** called `aus_domain` that was created above:

```
create-material aus_material
set-material-property aus_material G D aus_domain
$ [g]eneral properties: [d]omain
```

Then set the diffusion coefficient. Here, a user-specified value is used, instead of one calculated using information from the database, to better facilitate comparison with the analytical solution. The diffusion coefficient is stored in a variable for later use. The syntax below means [d]iffusion [c]oefficient of [c]arbon, [f]unction or expression.

```
set-variable-value diffCoeff 1e-12

set-material-property aus_material D C C F diffCoeff

${d}iffusion [c]oefficient of [c]arbon, [f]unction or expression
```

Following this, assign properties to the cells. Using the syntax below, the material `aus_material` is attached to all the cells.

```
set-cell-property a m aus_material ${a}ll cells, [m]aterial
```

Set the temperature of all cells to 1000°C, by first specifying that the temperatures should be in °C:

```
set-simulation-parameter N Y
```

specifying the temperature in the form of a variable:

```
set-variable-value sim_temp 1000
```

and then attaching this temperature property to all cells:

```
set-cell-property a V T sim_temp $ [a]ll cells, [v]ariable, [t]emperature
```

Assign the lower carbon content, `c_comp_bar`, to all cells.

```
set-cell-property a V C C c_comp_bar

$ [a]ll cells, [v]ariable, [c]omposition [c]arbon
```

The next stage is to select the cell in the middle of the bar using its cell index. First, we note that the first cell has the index 0, so the highest cell index in the array obtained using:

```
set-variable-value max_cell_index num_cells_x-1
```

and the index of the cell in the middle is given by:

```
set-variable-value middle_cell_index max_cell_index/2
```

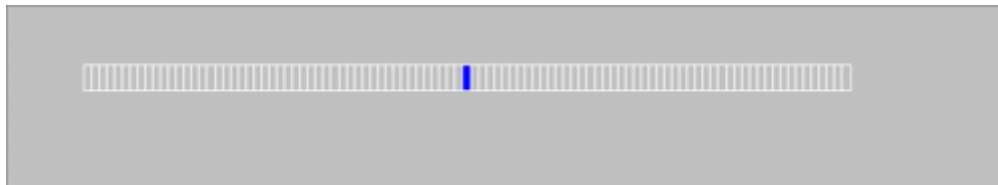
Then select the cell in the centre by its cell index:

```
add-cell-selection E middle_cell_index $ select the cell in the centre.
```

Assign the higher carbon content, `c_comp_layer`, to the selected cell (denoted by an asterisk).

```
set-cell-property * V C C c_comp_layer
```

The g5 window shows, by default, the selected cell(s) in blue:



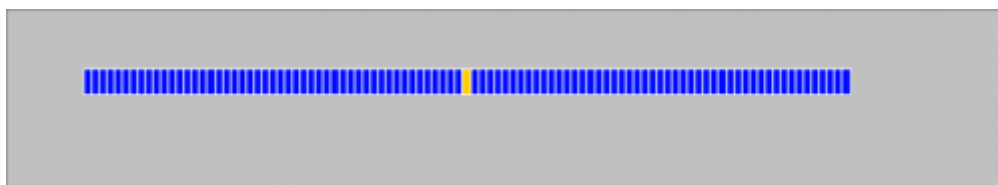
DISPLAY

The next stage is to set up the graphical display to look at the results. Firstly, assign a property to the existing paint window created above, `paint_window_id` so that the cells are coloured according to their carbon content.

```
set-gui-window-property paint_window_id I W V $ display cell variable
set-gui-window-property paint_window_id I V _cwp$c $ set which variable
set-gui-window-property paint_window_id I R 0..1
```

In the first line in the code above, the syntax represents s[i]mulation results, display [w]hat, [v]ariable. In the second, the [v]ariable is specified as `_cwp$c`, and in the third, the [r]ange is specified. The variable syntax `_cwp$c` represents the set of values of `wp$c` (weight percent of carbon) in the cells. Variables of this type can be found in the **variables** window under **cafe: cells**.

The cell array is shown schematically below, where blue represents a lower carbon content, and yellow a higher.



In addition, make a profile plot of the carbon content. Create a window of type **g1: plot grid: 1D profile**.

```
new-gui-window g1
```

Assign a name to both the plot window and the plot itself:

```
set-variable-value profile_window_id active_frame_id
```

```
set-variable-value profile_plot_id last_plot_id
```

Add a [s]eries, [n]ew of the [s]imulation variable `_cwp$c`.

```
set-plot-option profile_plot_id S N S _cwp$c
```

Specify that the default x-axis should be used, and give it a title:

```
set-gui-window-property profile_window_id S U Y  
set-gui-window-property profile_window_id S T Position [m]
```

Label the y-axis and specify its range:

```
set-plot-option profile_plot_id A Y 1 T Carbon content [wt.%]  
set-plot-option profile_plot_id A Y 1 S 0..c_comp_layer_wp
```

Give the plotted series the name 'Numerical':

```
set-plot-option profile_plot_id S M 0 Numerical
```

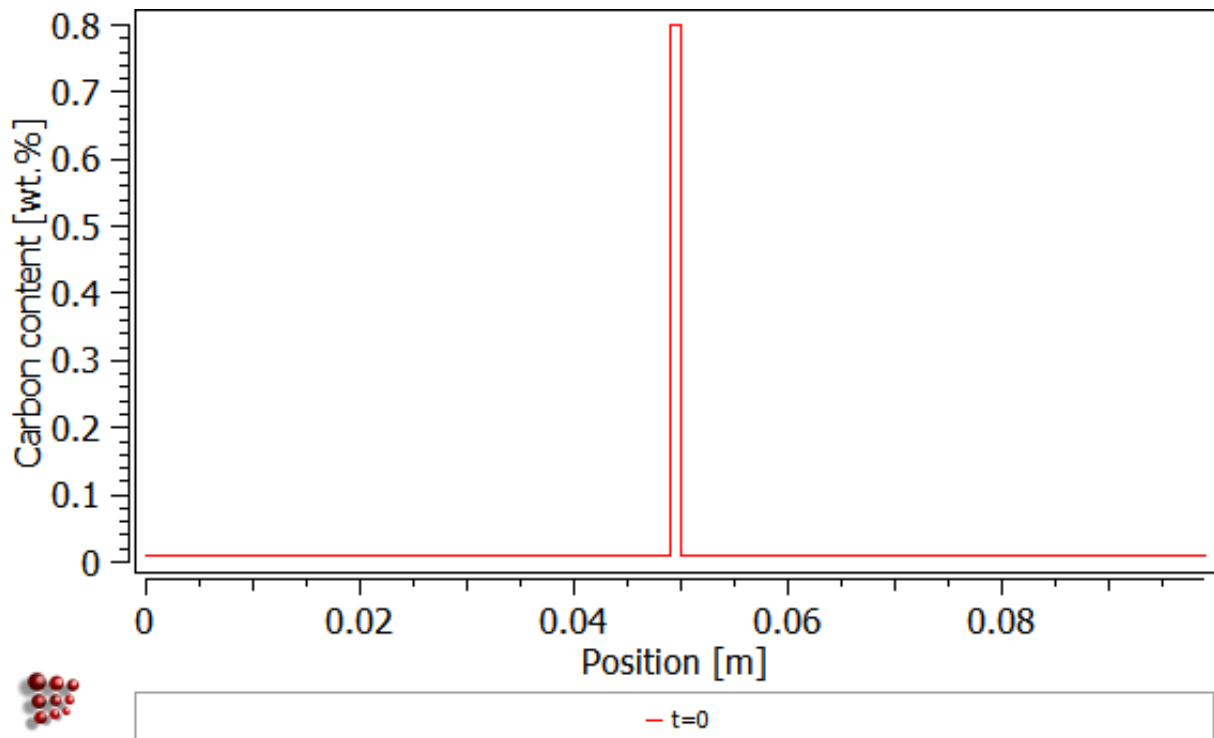
Specify the range of cells over which the profile is to be taken. In the syntax here, the first line gives the index of the s[t]arting cell (here 0) and the second line gives the index of the st[o]p cell (here `max_cell_index`).

```
set-gui-window-property profile_window_id I t 0  
set-gui-window-property profile_window_id I o max_cell_index
```

Give the window an appropriate size:

```
move-gui-window profile_window_id 20 20 600 400
```

The plot should look as shown:



We will now create a third window to display the time-dependent evolution of the carbon concentration in selected cells. The required window type is **g2: Plot grid: cell history**. Create the window and assign a name to the window and plot.

```
new-gui-window g2
set-variable-value history_window_id active_frame_id
set-variable-value history_plot_id last_plot_id
```

Use the following commands to specify that the default x-axis should be used and to assign it a title and a range.

```
set-gui-window-property history_window_id S U Y $use default x-axis
set-gui-window-property history_window_id S T Time [s]
set-gui-window-property history_window_id S S 0..sim_time
```

Label the y-axis and specify its range:

```
set-plot-option history_plot_id A Y 1 T Carbon content [wt. %]
set-plot-option history_plot_id A Y 1 S 0..c_comp_layer_wp
```

Now add two series, firstly the composition of the middle cell, and then that of the cell adjacent to it.

```
set-plot-option history_plot_id S N S _cwp$c{middle_cell_index}
set-plot-option history_plot_id S N S _cwp$c{middle_cell_index-1}
```

Give these series titles. Note that the quotation marks are needed for a multi-word title, as in the case of the series 'next to centre'

```
set-plot-option history_plot_id S M 0 centre
set-plot-option history_plot_id S M 1 'next to centre'
```

Finally, resize and move the history plot.

```
move-gui-window history_window_id 800 20 600 400
```

ANALYTICAL SOLUTION

In the final stage before setting up and running the simulation, the analytical solution will be added to the existing profile plot. Since the expression is rather complicated, it will be divided up into simpler terms:

$B_{val} * term_1 * term_2$

where B_{val} represents the integral giving the amount of solute in the system:

$$B = \int_{-\infty}^{\infty} C\{x, t\} dx,$$

$term_1$ is the term

$$\frac{1}{2\sqrt{\pi Dt}}$$

and $term_2$ is the term

$$\exp\left(\frac{-x^2}{4Dt}\right)$$

The value of the term B can be estimated by assuming that the initial concentration of carbon in the bar is small enough to be neglected, such that initially all the carbon is in the layer in the middle of the bar. The value of B is then simply the carbon concentration in the layer (in the units in which the curve is to be plotted, here weight percent, $c_comp_layer_wp$), multiplied by the width of the layer. The layer is one cell wide, i.e. the bar length divided by the number of cells.

```
set-variable-value Bval c_comp_layer_wp*(barlength/num_cells_x)
```

The cell variables (prefixed with `_c`) that we have seen earlier in this tutorial can be included in variables and functions. For example, `term_1` uses the cell variable `_ctime` to represent the time in the cell simulation. The variable `diffCoeff` was defined above, and `pi` is a built-in variable. (For details of the built-in variables of MatCalc, consult the section of the Reference Book on internal variables.)

```
set-function-expression term_1 1/(2*sqrt(pi*diffCoeff*_ctime))
```

It should be noted that the term x in the mathematical formulation of the analytical expression is measured from the centre of the range, whereas the cell variable corresponding to the x -position of the centre of the cells, `_ccenter_x`, is measured from the left-hand side of the system. We must therefore create an expression for the shifted x -coordinate:

```
set-variable-value midpt barlength/2
set-function-expression x_shifted _ccenter_x-midpt
set-function-expression term_2 exp((-1*x_shifted**2)/(4*diffCoeff*_ctime))
```

The analytical expression is then given by:

```
set-function-expression analytical_expr Bval*term_1*term_2
```

and this series is plotted onto the existing profile plot using the command:

```
set-plot-option profile_plot_id S N F analytical_expr 0..barlength
```

The `0..barlength` expression in the command above represents the range over which the function is to be evaluated; this corresponds to the length of the bar.

Note that when the analytical expression is first plotted, it looks slightly strange. This is because the time is initially zero, leading to a value of zero in the denominator of the first term, `term_1`.

SETTING UP AND RUNNING THE SIMULATION

The final set of commands deals with the simulation time and temperature, boundary conditions, type of simulation and update interval.

```
set-simulation-parameter e sim_time $ end
```

Specify the update interval:

```
set-simulation-parameter u 10 $ update interval
```

It is now necessary to tell the simulation module what type of problem should be simulated, i.e. how temperature and diffusion should be treated. In this case, we wish to simulate a **diffusion-field problem**, in which the elements are allowed to diffuse through the system:

```
set-simulation-parameter d f $ diffusion-field simulation
```


The temperature control, by contrast, is set to be isothermal and the hold temperature specified in terms of the variable `sim_temp` set earlier.

```
set-simulation-parameter t i sim_temp $ temperature: isothermal
```

The final step is to set up the default boundary conditions, i.e. the boundary conditions that apply in the absence of any other boundary conditions being set for specific cells or groups of cells. The type of boundary condition required is [g]eometric, and is set to [o]pen to environment. This means that there is no periodicity or symmetry.

```
set-default-boundary-cond G O $ open to environment.
```

Save the script.

To run the script, click on **Script > Run Script**, press **Shift + F2** or click on the  button. Then select the name of the script you wish to run from the drop-down menu and click on **Go**.

When the script has been correctly executed, select **Simulation > Start simulation** or press **Ctrl + J** to start the simulation. Output will appear in the Console, starting with:

```
#####

starting microstructure simulation ...

#####
```

and finishing with:

```
#####
#####
```



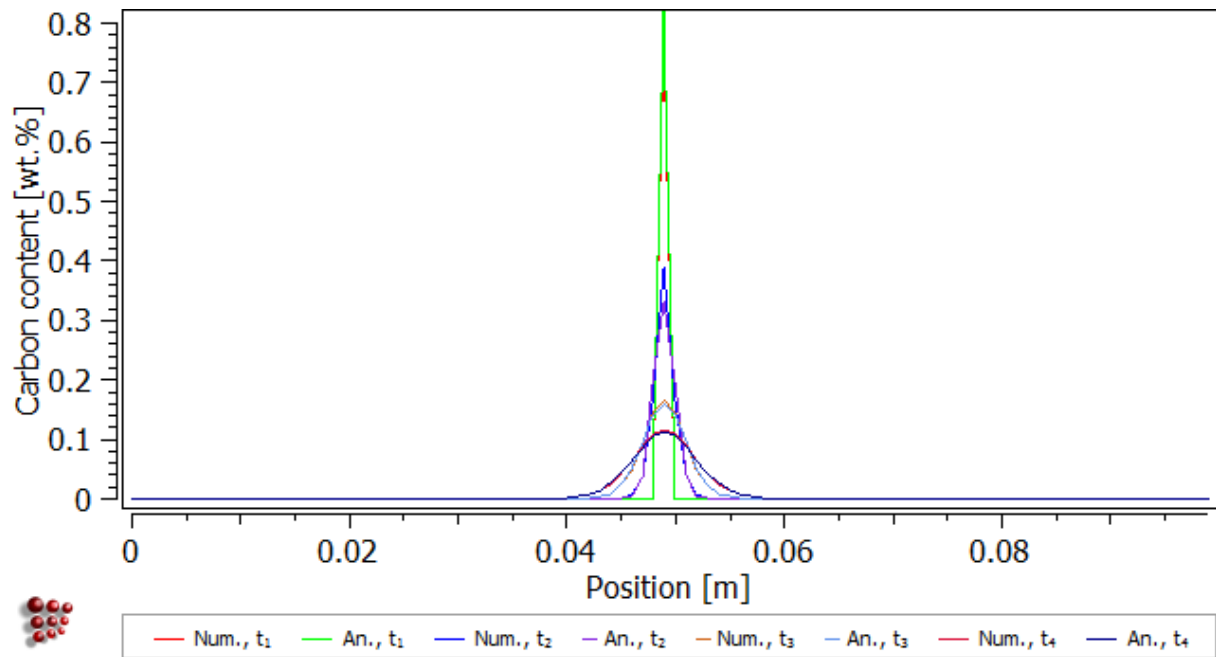
```
microstructure simulation finished in 59.07 secs (tot 59.07 secs) on Fri, 2016-06-10, 17:57:34
```

```
#####  
#####
```

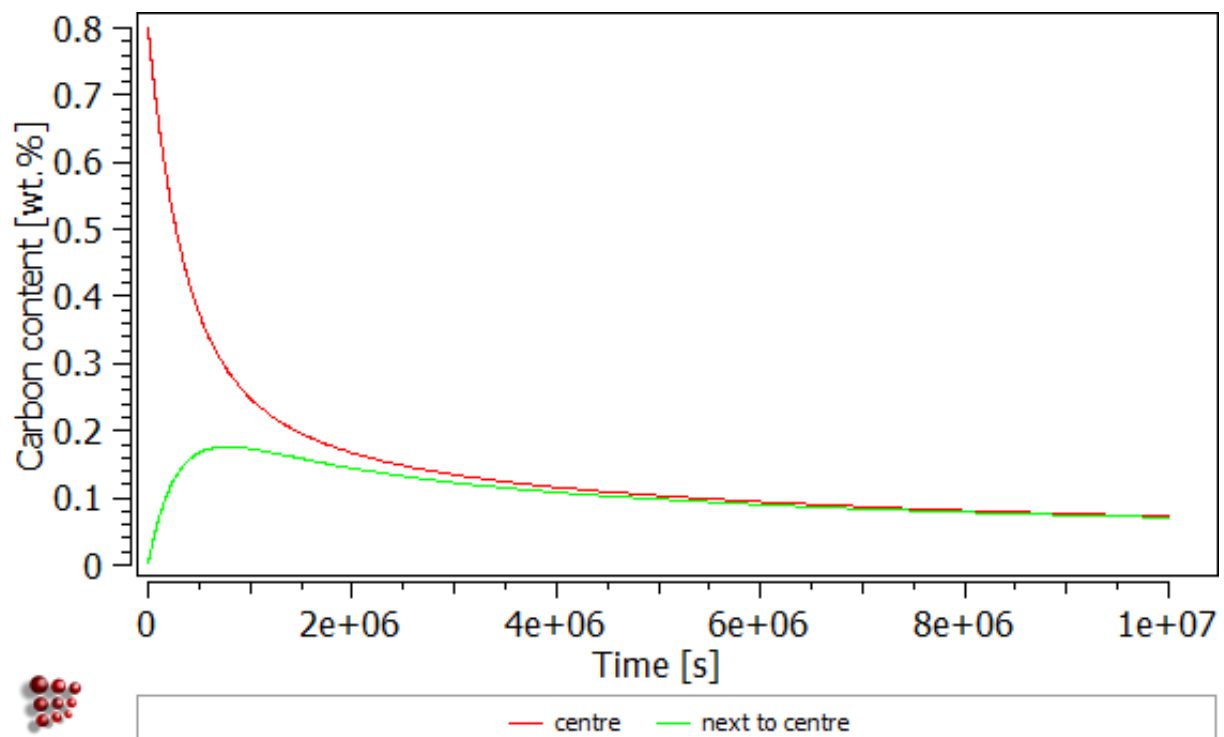
INTERPRETING THE RESULTS

You will notice that, at first, the peak value of the analytical expression is much higher than the maximum value of 0.8 wt. % in the numerical simulation. The reason for this is that the analytical solution is based on the assumption that all the carbon is initially in an infinitesimally thin layer, whereas in the numerical solution, we have put the carbon into a cell of finite thickness. As the simulation proceeds, the two curves start to approach each other until they eventually almost exactly coincide. By default, the profile plot is set to show a 'stepped' profile in which the concentration is shown as discrete values corresponding to the single concentration value assigned to each cell. In the **options** window for this plot, select **no** under **use steps** to instead see a smooth curve that may enable easier comparison with the analytical curve.

When the simulation is finished, you can examine the profiles at different times by looking at **Global > Buffers > Edit Buffer States**. You can obtain a set of profiles as shown below by loading up selected buffer states and using 'Duplicate and Lock all Series' on the plot right-click menu.



On the cell history plot, you should be able to see how the carbon concentration of the central cell decreases, while that of the adjacent cell decreases, until at longer exposure times, they converge.



APENDIX A

Related MatCalc scripts

SCRIPT TUTORIAL 2

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for calculation of a single equilibrium according to Tutorial 2.
 The following contents will be covered:

- 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

Database: mc_fe.tdb
 Author: P. Warczok
 Creation date: 20.03.2008
 Last update: 09.05.2019 (P. Warczok, Update for 6.02)
 This is a script for MatCalc version 6.02 (rel 1.003)

Known issues:

- "save-workspace "file-name"=Tutorial_2" is not working properly. Use "save-workspace Tutorial_2" instead.

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module module-name=core \$ select core module for kinetic simulation

close-workspace options=f \$ close any open workspace. Option "f" -> "force", does not ask for saving an open workspace

new-workspace \$ creates a new workspace

\$ Add some information about your Script

@ echo value=no

set-workspace-info information=+ This script reproduces all operations performed in Tutorial 2.

set-workspace-info information=+ I assumed it to be the first MatCalc script you are reading.

set-workspace-info information=+ Therefore, I tried to explain every new command which is given.

set-workspace-info information=+ Every line starting with "\$" contains a comment to a command.

set-workspace-info information=+ More information on scripting is given in Tutorial 13.

set-workspace-info information=+ Do not be afraid of scripting - this is much easier as you may think!

set-workspace-info This script reproduces all operations performed in Tutorial 2.

echo value=yes

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$$*****
      DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES
*****$$

$ Open database containing thermodynamic data
open-thermodynamic-database file-name=mc_fe.tdb
$ Select Fe, C and VA (vacancies) as components of the system.
$ VA is always selected as default, so it is actually not necessary to define it explicitly
$ FE is always selected as default in mc_fe.tdb, so it is actually not necessary to define it explicitly, either
select-elements elements=fe c va
$ Select the phases which will be used in the simulation
select-phases phases=liquid fcc_a1 bcc_a2 cementite graphite
$ Read data for the selected phases and elements from the database
read-thermodynamic-database

$ Set Fe as reference element
set-reference-element element=fe
$ Set the content of C to 0,4 wt.%
enter-composition type=weight-percent composition=c=0,4

$$*****
      EQUILIBRIUM CALCULATIONS
*****$$

$ Set the system temperature to 700°C
set-temperature-celsius temperature=700
$ Set the start values - this should prevent from any troubles in the equilibrium calculation
set-automatic-startvalues
$ Perform the equilibrium calculation
calculate-equilibrium

$----- Calculation with the suspended graphite phase -----$
$ Suspend graphite phase - a 'suspended' flag is set
change-phase-status phase-name=graphite set-flag=suspended
calculate-equilibrium

$----- Calculation graphite phase with zero phase fraction -----$
$ Activate graphite phase - a 'suspended' flag is cleared
change-phase-status phase-name=graphite clear-flag=suspended
$ Fix the phase fraction of graphite - a 'fixed' flag is set
change-phase-status phase-name=graphite set-flag=fixed
$ Set value of graphite phase fraction to '0' (zero)
change-phase-status phase-name=graphite mole-fraction-of-phase=0
calculate-equilibrium

$----- Calculation with the graphite phase removed -----$
$ Remove graphite phase
remove-phase phase-name=graphite
calculate-equilibrium

$----- Introducing graphite phase again -----$
$----- (requires a renewed selection of the phase in database) -----$

open-thermodynamic-database file-name=mc_fe.tdb
select-elements elements=fe c va
select-phases phases=liquid fcc_a1 bcc_a2 cementite graphite
read-thermodynamic-database

```

```
set-reference-element element=fe
enter-composition type=weight-percent composition=c=0,4
```

```
set-temperature-celsius temperature=700
set-automatic-startvalues
calculate-equilibrium
```

```
$$*****
```

CALCULATION STATES

```
*****$$
```

```
$ Create calculation state "Equil@700"
create-calc-state new-state-name=Equil@700
```

```
$ Calculation state for 600C
set-temperature-celsius temperature=600
calculate-equilibrium
create-calc-state new-state-name=Equil@600
```

```
$$*****
```

SAVING WORKSPACE

```
*****$$
```

```
$ Save workspace as "Tutorial_2.mcw"
$save-workspace "file-name"=Tutorial_2
save-workspace Tutorial_2
```

SCRIPT TUTORIAL 3

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for stepped equilibrium calculations according to Tutorial 3.
 The following contents will be covered:

- 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

Database: mc_fe.tdb

Author: P. Warczak

Creation date: 20.03.2008

Last update: 10.05.2019 (P. Warczak, Update for 6.02)

This is a script for MatCalc version 6.02 (rel 1.003)

Known issues:

- "save-workspace "file-name"=Tutorial_3" is not working properly. --> Use "save-workspace Tutorial_3" instead.
- A command "list-buffer-contents" is available which seems to be intended to double the command "list-calc-buffer-contents"
 --> Watch out in the next versions!

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module module-name=core \$ Use "core" module (MatCalc uses "core" module by default anyway)

read-workspace file-name=Tutorial_2.mcw \$ Loads the workspace "Tutorial_2.mcw"

```

$$*****
***** STEPPED EQUILIBRIUM CALCULATIONS *****
*****
  
```

\$----- Stepped equilibrium calculation with varying of temperature -----\$

\$ Select the calculation state "Equil@600" (this state is already selected by default)

select-calc-state Equil@600

\$ Load the data from the selected calculation state

load-calc-state calc-state-name=Equil@600

\$ Remove graphite phase

remove-phase graphite

\$ Select the type of calculation: Temperature variation

set-step-option type=temperature

\$ Define the range of the calculation: from 1600 to 400 with linear step of 25

set-step-option range start=1600 stop=400 scale=lin step-width=25

\$ Set the temperature unit to degree Celsius (instead of default Kelvin)

set-step-option temperature-in-celsius=yes

\$ Perform stepped equilibrium calculation

step-equilibrium

\$ Rename the current buffer to "T=400_to_1600°C"

rename-current-buffer new-buffer-name="T=400 to 1600°C"

```
$ Create a new buffer "C=0_to_1.5_at_500°C"
create-calc-buffer new-buffer-name="C=0 to 1.5 at 500°C"
```

```
$----- Stepped equilibrium calculation with varying carbon content - part I -----$
$ Select the type of calculation: Element content variation
set-step-option type=element-content
$ Define the range of the calculation: from 0 to 1.5 with linear step of 0.05
set-step-option range start=0 stop=1,5 scale=lin step-width=0,05
$ The temperature unit is degree Celsius, again.
set-step-option temperature-in-celsius=yes
$ Set temperature of the calculation to 500
set-step-option temperature=500
$ Global composition is varied - the "vary para-equilibrium constraints" option is deactivated
set-step-option vary-para-equil-constraints=no
$ Composition range is expressed in weight percent
set-step-option element-content-in-wt%=yes
```

```
step-equilibrium          $ Performs stepped equilibrium calculation
```

```
$----- Stepped equilibrium calculation with varying carbon content - part II -----$
```

```
$ Creating new buffer "C=0_to_1.5_at_800°C"
create-calc-buffer new-buffer-name="C=0 to 1.5 at 800°C"
```

```
$ Select the type of calculation: Element content variation
set-step-option type=element-content
$ Define the range of the calculation: from 0 to 1.5 with linear step of 0.05
set-step-option range start=0 stop=1,5 scale=lin step-width=0,05
set-step-option temperature-in-celsius=yes
$ Set temperature of the calculation to 500
set-step-option temperature=800
$ Global composition is varied - the "vary para-equilibrium constraints" option is deactivated
set-step-option vary-para-equil-constraints=no
$ Composition range is expressed in weight percent
set-step-option element-content-in-wt%=yes
$ Perform stepped equilibrium calculation
step-equilibrium
```

```
$$*****
      OPERATION ON BUFFER STATES
*****$$
```

```
$ Select the buffer state to edit
select-calc-buffer buffer-name="C=0 to 1.5 at 800°C"
```

```
$ List the contents of the selected buffer
list-calc-buffer-contents
```

```
$ Load the buffer state no.8
load-buffer-state line-index=8
```

```
$$*****
      SAVING WORKSPACE
*****$$
```

```
$ Save workspace as "Tutorial_3.mcw"
$save-workspace "file-name"=Tutorial_3
save-workspace Tutorial_3
```

SCRIPT TUTORIAL 4

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for graphical presentation and export of results according to Tutorial 4.
 The following contents will be covered:

- 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

Database: mc_fe.tdb
 Author: P. Warczok
 Creation date: 20.03.2008
 Last update: 10.05.2019 (P. Warczok, Update for 6.02)
 This is a script for MatCalc version 6.02 (rel 1.003)

Known issues:

- "save-workspace "file-name"=Tutorial_4" is not working properly. --> Use "save-workspace Tutorial_4" instead.

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module module-name=core \$ Use "core" module (MatCalc uses "core" module by default anyway)

read-workspace file-name=Tutorial_3.mcw \$ Loads the workspace "Tutorial_3.mcw"

select-calc-buffer buffer-name="T=400 to 1600°C"
 \$select-calc-buffer T=400_to_1600°C \$ Selects the buffer state to edit

```

$$*****
***** PLOTTING A GRAPH *****
*****
  
```

new-gui-window type-id=p1 \$ Creating a new window of 'p1' type (XY-diagram)
 \$ In plot no. 1, new series with buffer result for "f\$" -variables are plotted
 set-plot-option plot-id=1 series new buffer variable-name=f\$*

\$----- Results from different buffers -----
 \$ In the GUI window with id=2 (plot window), the content of the buffer "C=0 to 1.5 at 500°C" is plotted
 set-gui-window-property window-id=2 buffer-name="C=0 to 1.5 at 500°C"

\$ In the current window (described with "."), the content of the buffer "C=0 to 1.5 at 800°C" is plotted
 set-gui-window-property window-id=. buffer-name="C=0 to 1.5 at 800°C"

\$----- Changing the format of the temperature-step plot -----
 set-gui-window-property window-id=. buffer-name="T=400 to 1600°C" \$ Back to "T=400_to_1600C" buffer
 set-gui-window-property window-id=. default-x-axis-data=t\$c \$ Setting x-axis variable to temperature in "°C" (T\$c)
 set-gui-window-property window-id=. style-sheet=b/w \$ Changing the plot style to black and white (b/w)
 set-gui-window-property window-id=. style-sheet=col_no_symb \$... and back to colour

\$----- Setting title -----
 \$ Plot no.1 receives title "Phase fraction versus temperature for Fe-0.4 wt.%C"

set-plot-option plot-id=1 plot-title=Phase fraction versus temperature for Fe-0.4 wt.%C

\$----- Options for the plot legend -----

\$ For the current plot, the legend box is put on the bottom of the plot

set-plot-option plot-id=. legend-alignment=bottom

\$ For the current plot, the style of the legend frames is set to "none" (no frames displayed)

set-plot-option plot-id=. style=none

\$----- Options for the axes -----

\$ For the current plot, the x-axis becomes a title "Temperature [°C]"

set-plot-option plot-id=. x-axis-title=Temperature [°C]

\$ For the current plot, the y-axis becomes a title "Phase fraction"

set-plot-option plot-id=. y-axis-title=Phase fraction

\$ For the current plot, the y-axis scale type is set to logarithmic

set-plot-option plot-id=. y-axis-type=log

\$... and the scale range will start from 0.01

set-plot-option plot-id=. y-axis-scaling=0,01..

\$ To see the changes on the x-axis, the option of default x-axis usage for all plots is deactivated

set-gui-window-property window-id=. default-x-axis-for-all-plots=no

\$----- Options for the gridlines -----

\$ For the current plot, the major grids for the x-axis are enabled

set-plot-option plot-id=. grid which-grid=major enable-x-axis=yes

\$... together with the ones for the y-axis

set-plot-option plot-id=. grid which-grid=major enable-y-axis=yes

\$----- Options for the series -----

\$ The series no.0 of the current plot is renamed to "Liquid"

set-plot-option plot-id=. series rename series-index=0 new-name=Liquid

\$ The series no.1 of the current plot is renamed to "Austenite"

set-plot-option plot-id=. series rename series-index=1 new-name=Austenite

\$ The series no.2 of the current plot is renamed to "Ferrite"

set-plot-option plot-id=. series rename series-index=2 new-name=Ferrite

\$ The series no.3 of the current plot is renamed to "Cementite"

set-plot-option plot-id=. series rename series-index=3 new-name=Cementite

\$\$*****

SAVING WORKSPACE

*****\$\$

\$save-workspace "file-name"=Tutorial_4

\$ Saves workspace as "Tutorial_4.mcw"

save-workspace Tutorial_4

SCRIPT TUTORIAL 5

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for MatCalc built-in variables and graphical output according to Tutorial 5.
The following contents will be covered:

- 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

Database: mc_fe.tdb
Author: P. Warczok
Creation date: 20.03.2008
Last update: 10.05.2019 (P. Warczok, Update for 6.02)
This is a script for MatCalc version 6.02 (rel 1.003)

Known issues:

- "save-workspace "file-name"=Tutorial_5" is not working properly. --> Use "save-workspace Tutorial_5" instead.

```

*****
***** SETUP INFORMATION *****
*****
  
```

```

use-module module-name=core          $ Use "core" module (MatCalc uses "core" module by default anyway)

read-workspace file-name=Tutorial_4    $ Loads the workspace "Tutorial_4.mcw"
  
```

```

$$*****
***** ADDING PLOTS OF DIFFERENT VARIABLES *****
*****
  
```

\$ Creating new x-y plot in GUI-window no.2 (the number can read on the window bar)
create-new-plot plot-type=xy-plot attach-to-window=2

\$ For current ("." stands for "last used") plot a new series for buffer stored values of variable "dfm\$" is plotted
set-plot-option plot-id=. series new buffer variable-name=dfm\$*

\$----- Examples of other plots (every plot is plotted in a separate window) -----\$
create-new-plot plot-type=xy-plot attach-to-window=. \$ Creating new x-y plot in current GUI-window ("." stands for "last used")
set-plot-option plot-id=. series new buffer variable-name=gmp\$* \$ "gmp\$" -Molar Gibbs energy of various phases

\$ Chemical potential of carbon
create-new-plot plot-type=xy-plot attach-to-window=. \$ Creating new x-y plot in current GUI-window
set-plot-option plot-id=. series new buffer variable-name=mup\$*\$c \$ "mup\$*\$c" - Chemical potential of carbon in various phases

```
$ Molar heat capacity
create-new-plot plot-type=xy-plot attach-to-window=.
set-plot-option plot-id=. series new buffer variable-name=cpp$* $ "cpp$*" - Molar heat capacity of various phases
```

```
$ Arranging plots in two columns
set-gui-window-property window-id=. number-of-plot-columns=2
```

```
$----- Changing standard x-axis settings -----$
$ Default x-axis is to be used for all plots
set-gui-window-property window-id=. default-x-axis-for-all-plots=yes
$ Temperature in °C will be shown on the default x-axis
set-gui-window-property window-id=. default-x-axis-data=t$c
$ Setting the title for the default x-axis
set-gui-window-property window-id=. default-x-axis-title=Temperature [°C]
```

```
$$*****
MODIFYING THE SERIES IN PLOTS
*****$$
```

```
$----- Carbon concentration in the different phases -----$
create-new-plot plot-type=xy-plot attach-to-window=.
set-plot-option plot-id=. series new buffer variable-name=x$*$c $ "x$*$c" - mole fraction of C in various phases
```

```
$$ ----- The modification of carbon concentration from mole fractions -----
----- to weight percent - removing the old series and adding the new ones -----$$
$ Remove all series (all series meant with "*" in plot no.6
set-plot-option plot-id=6 series remove *
$ Plot "x$*$c$wp" - weight percent of C in various phases
set-plot-option plot-id=. series new buffer variable-name=x$*$c$wp
$ Y-axis gets the title "Carbon content of phase [wt.%]"
set-plot-option plot-id=. y-axis-title=Carbon content of phase [wt.%]
```

```
$$*****
SAVING WORKSPACE
*****$$
```

```
$save-workspace "file-name"=Tutorial_5 $ Saves workspace as "Tutorial_5.mcw"
save-workspace Tutorial_5
```

SCRIPT TUTORIAL 6

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for Introduction to user-defined functions and variables according to Tutorial 6.
 The following contents will be covered:

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

Database: mc_fe.tdb
 Author: P. Warczok
 Creation date: 20.03.2008
 Last update: 13.05.2019 (P. Warczok, Update for 6.02)
 This is a script for MatCalc version 6.02 (rel 1.003)

Known issues:

- "save-workspace "file-name"=Tutorial_6" is not working properly. Use "save-workspace Tutorial_6" instead.
- "set-gui-window-property window-id=. default-x-axis-legend=right" is not working for the plots created afterwards. If needed, use it after all plots are created in the given GUI-window.

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module module-name=core \$ Use "core" module (MatCalc uses "core" module by default anyway)

new-workspace \$ creates a new workspace

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****
  
```

open-thermodynamic-database file-name=mc_fe.tdb \$ Opens thermodynamic database mc_fe.tdb
 select-elements elements=FE C VA \$ Selects Fe and C as components of the system.
 \$ Select the phases which will be used in the simulation
 select-phases phases=LIQUID FCC_A1 BCC_A2 CEMENTITE
 \$ Read data for the selected phases and elements from the database
 read-thermodynamic-database

set-reference-element element=FE \$ Fe is set as a reference element
 enter-composition type=weight-percent composition=C=0,1 \$ Sets the content of C to 0.1 wt.%

```

$$*****
***** EQUILIBRIUM CALCULATIONS *****
*****
  
```

```

set-temperature-celsius temperature=1000          $ Sets the system temperature to 1000C
$ Set the start values - this should prevent from any troubles in the equilibrium calculation
set-automatic-startvalues
calculate-equilibrium                             $ Performs the equilibrium calculation

set-step-option type=temperature                  $ Selects the type of calculation (temperature as step-
variable)
set-step-option range start=400 stop=1600 scale=lin step-width=25      $ The calculation range: 400 - 1600; linear step
25
set-step-option temperature-in-celsius=yes        $ Temperature in Celsius

step-equilibrium

$$*****
                CREATING PLOTS
*****$$

new-gui-window type-id=p1                        $ Creating a new window of 'p1' type (XY-diagram)

set-plot-option plot-id=. series new buffer variable-name=F$*          $ Plotting phase fractions
set-gui-window-property window-id=. default-x-axis-data=t$C            $ Temperature in Celsius on x-axis
set-gui-window-property window-id=. default-x-axis-title=Temperature [°C] $ Title of x-axis
$set-gui-window-property window-id=. default-x-axis-legend=right        $ the legend box is put on the right side

$$*****
                COMBINING BUILT-IN VARIABLES IN NEW EXPRESSIONS
*****$$

create-new-plot plot-type=xy-plot attach-to-window=.          $ new plot

$ The product of carbon content in liquid and phase fraction of liquid is plotted
set-plot-option plot-id=. series new buffer variable-name=X$LIQUID$C*$F$LIQUID
$ The product of carbon content in bcc and phase fraction of bcc is plotted
set-plot-option plot-id=. series new buffer variable-name=X$BCC_A2$C*$F$BCC_A2
$ The product of carbon content in fcc and phase fraction of fcc is plotted
set-plot-option plot-id=. series new buffer variable-name=X$FCC_A1$C*$F$FCC_A1
$ The product of carbon content in cementite and phase fraction of cementite is plotted
set-plot-option plot-id=. series new buffer variable-name=X$CEMENTITE$C*$F$CEMENTITE
$ The carbon content in the system is plotted
set-plot-option plot-id=. series new buffer variable-name=X$S$C

$$*****
                DEFINING FUNCTIONS
*****$$

$ Defining function "C_in_liquid" as a product of carbon content in liquid and phase fraction of liquid
set-function-expression function=C_in_liquid expression=X$LIQUID$C*$F$LIQUID
$ Defining function "C_in_bcc" as a product of carbon content in bcc and phase fraction of bcc
set-function-expression function=C_in_bcc expression=X$BCC_A2$C*$F$BCC_A2
$ Defining function "C_in_fcc" as a product of carbon content in fcc and phase fraction of fcc
set-function-expression function=C_in_fcc expression=X$FCC_A1$C*$F$FCC_A1
$ Defining function "C_in_cementite" as a product of carbon content in cementite and phase fraction of cementite
set-function-expression function=C_in_cementite expression=X$CEMENTITE$C*$F$CEMENTITE

$----- Plotting new functions instead of "X$...*$F$..." products -----$
$ Remove all (all is denoted with "*") series in the current plot
set-plot-option plot-id=. series remove series-index=*
set-plot-option plot-id=. series new buffer variable-name=C_in_liquid      $ Plotting "C_in_liquid"

```

```

set-plot-option plot-id=. series new buffer variable-name=C_in_bcc      $ Plotting "C_in_bcc"
set-plot-option plot-id=. series new buffer variable-name=C_in_fcc      $ Plotting "C_in_fcc"
set-plot-option plot-id=. series new buffer variable-name=C_in_cementite $ Plotting "C_in_cementite"
set-plot-option plot-id=. series new buffer variable-name=XS$C          $ Plotting carbon content in the system

```

```

$----- Defining and plotting new expressions using existing functions -----$
$ Defining a function "Fraction_C_in_liquid" as C_in_liquid divided by molar fraction of carbon
set-function-expression function=Fraction_C_in_liquid expression=C_in_liquid/XS$C
$ Defining a function "Fraction_C_in_bcc" as C_in_bcc divided by molar fraction of carbon
set-function-expression function=Fraction_C_in_bcc expression=C_in_bcc/XS$C
$ Defining a function "Fraction_C_in_fcc" as C_in_fcc divided by molar fraction of carbon
set-function-expression function=Fraction_C_in_fcc expression=C_in_fcc/XS$C
$ Defining function "Fraction_C_in_cementite" as C_in_cementite divided by molar fraction of carbon
set-function-expression function=Fraction_C_in_cementite expression=C_in_cementite/XS$C

```

```

create-new-plot plot-type=xy-plot attach-to-window=.
set-plot-option plot-id=. series new buffer variable-name=Fraction_C_in_liquid $ Plotting "Fraction_C_in_liquid"
set-plot-option plot-id=. series new buffer variable-name=Fraction_C_in_bcc    $ Plotting "Fraction_C_in_bcc"
set-plot-option plot-id=. series new buffer variable-name=Fraction_C_in_fcc    $ Plotting "Fraction_C_in_fcc"
set-plot-option plot-id=. series new buffer variable-name=Fraction_C_in_cementite $ Plotting "Fraction_C_in_cementite"

```

```

$----- Displaying the results of the stepped calculation varying carbon content -----$
set-gui-window-property window-id=. default-x-axis-data=Stepvalue          $ Stepvalue on x-axis
set-gui-window-property window-id=. default-x-axis-title=C content [wt.%]   $ Changing the title of x-axis

```

```

set-step-option type=element-content          $ Varying element content
set-step-option range start=0 stop=0,5 scale=lin step-width=0,005          $ in range 0 - 0.5; linear step 0.005
set-step-option element=C                  $ The element is carbon
set-step-option temperature=1475           $ at 1475
set-step-option temperature-in-celsius=yes  $ in Celsius
set-step-option element-content-in-wt%=yes  $ and carbon content in wt.%
step-equilibrium

```

```

$$*****
USER-DEFINED VARIABLES
*****$$

```

```

set-variable-value variable=x1 value=0,27813585          $ Setting x1 = 0,27813585
set-variable-value variable=y1 value=0                   $ Setting y1 = 0
set-variable-value variable=x2 value=0.5                 $ Setting x2 = 0.5

```

```

$----- Finding the value of "y2"-variable -----$
enter-composition type=weight-percent composition=C=0,5    $ Carbon content = 0.5 wt.%
set-temperature-celsius temperature=1475                   $ Temperature = 1475C
calculate-equilibrium                                     $ Equilibrium calculation
set-variable-value variable=y2 value=C_in_liquid           $ Setting y2 = C_in_liquid

```

```

$ Defining the parameters of the function approximating the amount of carbon present in liquid phase
set-variable-value variable=a value=(y2-y1)/(x2-x1)        $ setting a (slope)
set-variable-value variable=b value=((x2*y1)-(x1*y2))/(x2-x1) $ setting b (intersection)
set-function-expression function=Liquid_line expression=(a*x)+b $ defining "Liquid_line"
set-plot-option plot-id=2 series new buffer variable-name=Liquid_line $ Plotting "Liquid_line" in plot no.2

```

```

$ Cutting off negative values of "Liquid_line" by setting the curve as a function/expression plot

```

set-gui-window-property window-id=. default-x-axis-legend=right \$ the legend box is put on the right side

```
$save-workspace "file-name"=Tutorial_6
save-workspace Tutorial_6
```

SCRIPT TUTORIAL 7

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for calculating phase boundaries according to Tutorial 7.
 The following contents will be covered:

- 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

Database: mc_fe.tdb
 Author: P. Warczok
 Creation date: 20.03.2008
 Last update: 14.05.2019 (P. Warczok, Update for 6.02)
 This is a script for MatCalc version 6.02 (rel 1.003)

Known issues:

- "save-workspace "file-name"=Tutorial_7" is not working properly. Use "save-workspace Tutorial_7" instead.
- Dependent phase for the stepped calculation of "phase boundary" type can be defined either by "set-step-option scheil-dependent-phase=" or by "set-step-option T0-dependent-phase=", though this is not "Scheil" or "T0" calculation... Still, both of these seem to work fine in this role as well.

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module module-name=core \$ Use "core" module (MatCalc uses "core" module by default anyway)

new-workspace \$ creates a new workspace

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****
  
```

open-thermodynamic-database file-name=mc_fe.tdb \$ Thermodynamic database: mc_fe.tdb
 select-elements elements=FE C NB VA \$ Components: Fe, C, Nb
 select-phases phases=LIQUID FCC_A1 BCC_A2 CEMENTITE \$ Phases: Liquid, fcc, bcc, cementite
 read-thermodynamic-database

set-reference-element element=FE
 enter-composition type=weight-percent composition=C=0,1 NB=0,3 \$ Composition: 0.1 wt.% C, 0.3 wt.% Nb

set-temperature-celsius temperature=1000
 set-automatic-startvalues
 calculate-equilibrium \$ Initial equilibrium

```

$$*****
***** CALCULATING PHASE BOUNDARIES *****
*****
  
```


\$----- Solidus and liquidus temperature -----\$

\$ Searching a phase boundary for the liquid phase field varying temperature

search-phase-boundary phase-name=LIQUID temperature

\$ Searching a phase boundary for the bcc phase field varying temperature

search-phase-boundary phase-name=BCC_A2 temperature

set-temperature-celsius temperature=1600

calculate-equilibrium

search-phase-boundary phase-name=BCC_A2 temperature

\$ Finding liquidus

\$----- Austenite-ferrite transformation temperatures -----\$

set-temperature-celsius temperature=700

calculate-equilibrium

search-phase-boundary phase-name=FCC_A1 temperature

\$ Phase boundary of fcc phase field

set-temperature-celsius temperature=900

calculate-equilibrium

search-phase-boundary phase-name=BCC_A2 temperature

\$ Phase boundary of bcc phase field

\$----- Dissolution temperatures of carbides -----\$

set-temperature-celsius temperature=800

calculate-equilibrium

search-phase-boundary phase-name=CEMENTITE temperature

\$ Phase boundary of cementite phase

field

set-temperature-celsius temperature=1200

calculate-equilibrium

search-phase-boundary phase-name=FCC_A1#01 temperature

\$ Phase boundary of NbC phase field

\$----- ELEMENT CONTENT FOR ZERO-PHASE FRACTIONS -----\$

\$----- C-content of cementite phase boundary at 700C -----\$

set-temperature-celsius temperature=700

calculate-equilibrium

\$ Searching a phase boundary for the cementite phase field varying element content.

\$ Carbon content will be varied at 700C ("Temperature in Celsius" is switched to yes)

search-phase-boundary phase-name=CEMENTITE element-content element=C temperature=700 temperature-in-C=yes

\$----- Nb-content of NbC phase boundary at 1000C -----\$

enter-composition type=weight-percent composition=C=0,1

\$ Resets the carbon content

set-temperature-celsius temperature=1000

calculate-equilibrium

\$ Searching a phase boundary for the NbC phase field varying element content.

\$ Nb content will be varied at 1000C ("Temperature in Celsius" is switched to yes)

search-phase-boundary phase-name=FCC_A1#01 element-content element=NB temperature=1000 temperature-in-C=yes

\$----- TRACING PHASE BOUNDARIES -----\$

\$----- NbC phase boundary for C-content of 0,1 wt.% -----\$

set-step-option type=phase-boundary

\$ Selects "Phase boundary" as calculation type

set-step-option range start=0,01 stop=0,35 scale=lin step-width=0,01

\$ Range 0,01 - 0,6; linear step of 0,01

set-step-option element=NB

\$ Niobium content varied

set-step-option T0-dependent-phase=FCC_A1#01

\$ Setting the max. T-step to 100

set-step-option maximum-temperature-step=100

set-step-option temperature-in-celsius=yes

\$ Temperature in Celsius

set-step-option element-content-in-wt%=yes

\$ Composition in wt.%

step-equilibrium

new-gui-window type-id=p1

\$ Creating plot

\$ Plotting the phase boundary (Temperature in C vs. Nb content)

```

set-plot-option plot-id=. series new buffer variable-name=T$C
$ For current plot ("."), series "T$C" is duplicated and locked
set-plot-option plot-id=. series duplicate-and-lock series-index=-1 series-name=T$c
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T$C new-name="0.1 wt.%C" $ Renames the series
"*_T$C" to "0.1 wt.%C"

$----- NbC phase boundary for C-content of 0,05 wt.% -----$
enter-composition type=weight-percent composition=C=0,05 $ C content = 0,05 wt.%
set-temperature-celsius temperature=1000
calculate-equilibrium

$ Search phase boundary of NbC phase field varying Nb content at 1000C
search-phase-boundary phase-name=FCC_A1#01 element-content element=NB temperature=1000 temperature-in-C=yes

set-step-option type=phase-boundary $ Selects the t[y]pe of calculation: "Phase boundary"
set-step-option range start=0,01 stop=0,35 scale=lin step-width=0,01 $ Range 0,01 - 0,6; linear step of 0,01
set-step-option element=NB $ Niobium content varied
set-step-option scheil-dependent-phase=FCC_A1#01 $ Phase boundary of NbC phase field
set-step-option maximum-temperature-step=100 $ Setting the max. T-step to 100
set-step-option temperature-in-celsius=yes $ Temperature in Celsius
set-step-option element-content-in-wt%=yes $ Composition in wt.%
step-equilibrium

$ For current plot ("."), series "T$C" is duplicated and locked
set-plot-option plot-id=. series duplicate-and-lock series-index=-1 series-name=T$c
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T$C new-name="0.05 wt.%C" $ Renames the series
"*_T$C" to "0.05 wt.%C"

$----- NbC phase boundary for C-content of 0,01 wt.% -----$
enter-composition type=weight-percent composition=C=0,01 $ C content = 0,01 wt.%
set-temperature-celsius temperature=1000
calculate-equilibrium

$ Searching phase boundary of NbC phase field varying Nb content at 1000C
search-phase-boundary phase-name=FCC_A1#01 element-content element=NB temperature=1000 temperature-in-C=yes

set-step-option type=phase-boundary $ "Phase boundary" type
set-step-option range start=0,01 stop=0,35 scale=lin step-width=0,01 $ Range 0,01 - 0,6; linear step of 0,01
set-step-option element=NB $ Niobium content varied
set-step-option scheil-dependent-phase=FCC_A1#01 $ Phase boundary of NbC phase field
set-step-option maximum-temperature-step=100 $ Setting the max. T-step to 100
set-step-option temperature-in-celsius=yes $ Temperature in Celsius
set-step-option element-content-in-wt%=yes $ Composition in wt.%
step-equilibrium

$ For current plot ("."), series "T$C" is locked (do-lock=yes)
set-plot-option plot-id=. series lock series-index=-1 series-name=T$c do-lock=yes
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T$C new-name="0.01 wt.%C" $ Renames the series
"*_T$C" to "0.01 wt.%C"

set-plot-option plot-id=. plot-title=Phase boundary of NbC $ Plot title
set-gui-window-property window-id=. default-x-axis-title=Nb content [wt.%] $ x-axis title - defined over default
x-axis settings
set-plot-option plot-id=. y-axis-title=Temperature [C] $ y-axis title
set-plot-option plot-id=. grid which-grid=major enable-x-axis=yes $ Plotting major grid lines for x-axis
set-plot-option plot-id=. grid which-grid=major enable-y-axis=yes $ Plotting major grid lines for y-axis

$$*****
$ SAVING WORKSPACE
*****$$

```

```
$save-workspace "file-name"=Tutorial_7
```

save-workspace Tutorial_7

SCRIPT TUTORIAL 8

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for calculating a phase diagram in a binary system according to Tutorial 8.
 The following contents will be covered:

- 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 (Fe₃C). 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 Fe₃C. In this tutorial, phase diagrams for both Fe-C and Fe-Fe₃C will be calculated.

Database: mc_fe.tdb
 Author: P. Warczok
 Creation date: 10.11.2008
 Last update: 15.05.2019 (P. Warczok, Update for 6.02)
 This is a script for MatCalc version 6.02 (rel 1.003)

Known issues:

- "save-workspace "file-name"=Tutorial_8" is not working properly. Use "save-workspace Tutorial_8" instead.
- Dependent phase for the stepped calculation of "phase boundary" type can be defined either by "set-step-option scheil-dependent-phase=" or by "set-step-option T0-dependent-phase=", though this is not "Scheil" or "T0" calculation... Still, both of these seem to work fine in this role as well.

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module module-name=core \$ Use "core" module (MatCalc uses "core" module by default anyway)

new-workspace \$ creates a new workspace

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****
  
```

```

open-thermodynamic-database file-name=mc_fe.tdb          $ Thermodynamic database: mc_fe.tdb
select-elements elements=FE C VA                        $ Components: Fe, C
select-phases phases=LIQUID FCC_A1 BCC_A2 CEMENTITE GRAPHITE $ Phase selection
read-thermodynamic-database
  
```

```

set-reference-element element=FE
enter-composition type=weight-percent composition=C=0,05 $ Composition: 0.05 wt.% C
  
```

```

set-automatic-startvalues
set-temperature-celsius temperature=1000                $ Temperature 1000C
calculate-equilibrium                                  $ Initial equilibrium

new-gui-window type-id=p1                               $ Plot of the phase diagram

$ Suspend graphite phase
change-phase-status phase-name=graphite set-flag=suspended

$$*****
FE-FE3C PHASE DIAGRAM
*****$$

$----- Upper boundary of delta-ferrite -----$
set-temperature-celsius temperature=1530                $ Temperature 1530C
calculate-equilibrium
search-phase-boundary phase-name=BCC_A2 temperature      $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                    $ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2           $ Phase boundary of bcc phase field
set-step-option element=C                               $ Carbon content varied
set-step-option range start=0 stop=5 scale=lin step-width=0.01 $ Range 0 - 5; linear step of 0,01
set-step-option element-content-in-wt%=yes              $ Composition in wt.%
set-step-option temperature-in-celsius=yes              $ Temperature in Celsius
set-step-option maximum-temperature-step=20            $ Setting the max. T-step to 20
step-equilibrium

set-plot-option plot-id=. series new buffer variable-name=T$C $ Plotting the phase boundary
$ Display major grid lines for x-axis
set-plot-option plot-id=. grid which-grid=major enable-x-axis=yes
$ Display major grid lines for y-axis
set-plot-option plot-id=. grid which-grid=major enable-y-axis=yes
$ Duplicate and lock all (unlocked) series
set-gui-window-property window-id=. duplicate-and-lock-plot-series
$ Renaming series: "*_T$C" -> "bcc_high_1"
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T$C new-name=bcc_high_1

$----- Lower boundary of liquid -----$
set-temperature-celsius temperature=1500                $ Temperature 1500C
calculate-equilibrium
search-phase-boundary phase-name=LIQUID temperature      $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                    $ "Phase boundary" type
set-step-option scheil-dependent-phase=LIQUID           $ Phase boundary of liquid phase field
set-step-option element=C                               $ Carbon content varied
set-step-option range start=0 stop=5 scale=lin step-width=0.01 $ Range 0 - 5; linear step of 0,01
set-step-option element-content-in-wt%=yes              $ Composition in wt.%
set-step-option temperature-in-celsius=yes              $ Temperature in C
set-step-option maximum-temperature-step=20            $ Setting the max. T-step to 20
step-equilibrium

$ Duplicate and lock all unlocked series
set-gui-window-property window-id=. duplicate-and-lock-plot-series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T$C new-name=liquid $ Renaming series: "*_T$C" -
-> "liquid"

$----- Lower boundary of delta-ferrite -----$

```

```

set-temperature-celsius temperature=1400                $ Temperature 1400C
calculate-equilibrium
search-phase-boundary phase-name=BCC_A2 temperature    $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                    $ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2          $ Phase boundary of bcc phase field
set-step-option element=C                             $ Carbon content varied
set-step-option range start=0 stop=5 scale=lin step-width=0.01 $ Range 0 - 5; linear step of 0,01
set-step-option element-content-in-wt%=yes             $ Composition in wt.%
set-step-option temperature-in-celsius=yes             $ Temperature in Celsius
set-step-option maximum-temperature-step=20           $ Setting the max. T-step to 20
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T$C new-name=bcc_high_2 $ Renaming series:
"*_T$C" -> "bcc_high_2"

$----- Upper boundary of austenite -----$
set-temperature-celsius temperature=1500                $ Temperature 1500C
calculate-equilibrium
search-phase-boundary phase-name=FCC_A1 temperature    $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                    $ "Phase boundary" type
set-step-option scheil-dependent-phase=FCC_A1          $ Phase boundary of fcc phase field
set-step-option element=C                             $ Carbon content varied
set-step-option range start=0 stop=5 scale=lin step-width=0.01 $ Range 0 - 5; linear step of 0,01
set-step-option element-content-in-wt%=yes             $ Composition in wt.%
set-step-option temperature-in-celsius=yes             $ Temperature in Celsius
set-step-option maximum-temperature-step=20           $ Setting the max. T-step to 20
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T$C new-name=fcc_1 $ Renaming series: "*_T$C" -
-> "fcc_1"

$----- Upper boundary of alpha-ferrite -----$
set-temperature-celsius temperature=900                $ Temperature 900C
calculate-equilibrium
search-phase-boundary phase-name=BCC_A2 temperature    $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                    $ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2          $ Phase boundary of bcc phase field
set-step-option element=C                             $ Carbon content varied
set-step-option range start=0 stop=5 scale=lin step-width=0.01 $ Range 0 - 5; linear step of 0,01
set-step-option element-content-in-wt%=yes             $ Composition in wt.%
set-step-option temperature-in-celsius=yes             $ Temperature in Celsius
set-step-option maximum-temperature-step=20           $ Setting the max. T-step to 20
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T$C new-name=bcc_low $ Renaming series: "*_T$C"
--> "bcc_low"

$----- Lower boundary of austenite -----$
set-temperature-celsius temperature=600                $ Temperature 600C
calculate-equilibrium

```

```

search-phase-boundary phase-name=FCC_A1 temperature          $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                          $ "Phase boundary" type
set-step-option scheil-dependent-phase=FCC_A1                $ Phase boundary of fcc phase field
set-step-option element=C                                    $ Carbon content varied
set-step-option range start=0 stop=5 scale=lin step-width=0.001 $ Range 0 - 5; linear step of 0,001
set-step-option element-content-in-wt%=yes                    $ Composition in wt.%
set-step-option temperature-in-celsius=yes                    $ Temperature in Celsius
set-step-option maximum-temperature-step=20                  $ Setting the max. T-step to 20
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T$C new-name=fcc_2 $ Renaming series: "*_T$C" -
-> "fcc_2"

$----- Cementite upper phase boundary -----$
set-temperature-celsius temperature=800                      $ Temperature 800C
calculate-equilibrium
search-phase-boundary phase-name=CEMENTITE temperature      $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                          $ "Phase boundary" type
set-step-option scheil-dependent-phase=CEMENTITE              $ Phase boundary of cementite phase field
set-step-option element=C                                    $ Carbon content varied
set-step-option range start=0 stop=5 scale=lin step-width=0.01 $ Range 0 - 5; linear step of 0,01
set-step-option element-content-in-wt%=yes                    $ Composition in wt.%
set-step-option temperature-in-celsius=yes                    $ Temperature in Celsius
set-step-option maximum-temperature-step=200                  $ Setting the max. T-step to 200
step-equilibrium

$ lock series "T$C"
set-plot-option plot-id=. series lock series-index=-1 series-name=T$C do-lock=yes
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T$C new-name=cementite $ Renaming series: "*_T$C"
--> "cementite"

$----- The finished diagram -----$
$ Plot title. "<sub>" and "</sub>" are used to mark the text which should be written as a subscript
set-plot-option plot-id=. plot-title=Fe-Fe<sub>3</sub>C phase diagram
set-gui-window-property window-id=. default-x-axis-title=Carbon content [wt.%] $ x-axis title
set-plot-option plot-id=. y-axis-title=Temperature [C] $ y-axis title
$ Scaling of y-axis starts from "400"
set-plot-option plot-id=. y-axis-scaling=400..

$$*****
FE-C PHASE DIAGRAM
*****$$

$ Activate graphite again - remove "suspended" flag
change-phase-status phase-name=GRAPHITE clear-flag=suspended
set-temperature-celsius temperature=1600                      $ Temperature 1600C
calculate-equilibrium

create-new-plot plot-type=xy-plot attach-to-window=.          $ Fe-C phase diagram will be drawn on the new
plot
set-plot-option plot-id=. grid which-grid=major enable-x-axis=yes $ Switching on the major gridlines for x-axis
set-plot-option plot-id=. grid which-grid=major enable-y-axis=yes $ Switching on the major gridlines for y-axis

$----- Upper boundary of delta-ferrite -----$

```

search-phase-boundary phase-name=BCC_A2 temperature
boundary search \$ Varying temperature for the phase

set-step-option type=phase-boundary \$ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2 \$ Phase boundary of bcc phase field
set-step-option element=C \$ Carbon content varied
set-step-option range start=0 stop=5 scale=lin step-width=0.01 \$ Range 0 - 5; linear step of 0,01
set-step-option element-content-in-wt%=yes \$ Composition in wt.%
set-step-option temperature-in-celsius=yes \$ Temperature in Celsius
set-step-option maximum-temperature-step=20 \$ Setting the max. T-step to 20
step-equilibrium

set-plot-option plot-id=. series new buffer variable-name=T\$C \$ Drawing the phase boundary in the new plot
set-gui-window-property window-id=. duplicate-and-lock-plot-series \$ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T\$C new-name=bcc_high_1 \$ Renaming series:
"*_T\$C" -> "bcc_high_1"

\$----- Lower boundary of liquid -----
set-temperature-celsius temperature=1500 \$ Temperature 1500C
calculate-equilibrium
search-phase-boundary phase-name=LIQUID temperature \$ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary \$ "Phase boundary" type
set-step-option scheil-dependent-phase=LIQUID \$ Phase boundary of liquid phase field
set-step-option element=C \$ Carbon content varied
set-step-option range start=0 stop=5 scale=lin step-width=0.01 \$ Range 0 - 5; linear step of 0,01
set-step-option element-content-in-wt%=yes \$ Composition in wt.%
set-step-option temperature-in-celsius=yes \$ Temperature in Celsius
set-step-option maximum-temperature-step=20 \$ Setting the max. T-step to 20
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series \$ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T\$C new-name=liquid \$ Renaming series: "*_T\$C" -
-> "liquid"

\$----- Lower boundary of delta-ferrite -----
set-temperature-celsius temperature=1400 \$ Temperature 1400C
calculate-equilibrium
search-phase-boundary phase-name=BCC_A2 temperature \$ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary \$ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2 \$ Phase boundary of bcc phase field
set-step-option element=C \$ Carbon content varied
set-step-option range start=0 stop=5 scale=lin step-width=0.01 \$ Range 0 - 5; linear step of 0,01
set-step-option element-content-in-wt%=yes \$ Composition in wt.%
set-step-option temperature-in-celsius=yes \$ Temperature in Celsius
set-step-option maximum-temperature-step=20 \$ Setting the max. T-step to 20
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series \$ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T\$C new-name=bcc_high_2 \$ Renaming series:
"*_T\$C" -> "bcc_high_2"

\$----- Upper boundary of austenite -----
set-temperature-celsius temperature=1500 \$ Temperature 1500C
calculate-equilibrium

search-phase-boundary phase-name=FCC_A1 temperature boundary search \$ Varying temperature for the phase

set-step-option type=phase-boundary \$ "Phase boundary" type
 set-step-option scheil-dependent-phase=FCC_A1 \$ Phase boundary of fcc phase field
 set-step-option element=C \$ Carbon content varied
 set-step-option range start=0 stop=5 scale=lin step-width=0.01 \$ Range 0 - 5; linear step of 0,01
 set-step-option element-content-in-wt%=yes \$ Composition in wt.%
 set-step-option temperature-in-celsius=yes \$ Temperature in Celsius
 set-step-option maximum-temperature-step=20 \$ Setting the max. T-step to 20
 step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series \$ Locking all unlocked series
 set-plot-option plot-id=. series rename series-index=-1 series-name=*_T\$C new-name=fcc_1 \$ Renaming series: "*_T\$C" -
 -> "fcc_1"

\$----- Upper boundary of alpha-ferrite -----\$
 set-temperature-celsius temperature=900 \$ Temperature 900C
 calculate-equilibrium
 search-phase-boundary phase-name=BCC_A2 temperature boundary search \$ Varying temperature for the phase

set-step-option type=phase-boundary \$ "Phase boundary" type
 set-step-option scheil-dependent-phase=BCC_A2 \$ Phase boundary of bcc phase field
 set-step-option element=C \$ Carbon content varied
 set-step-option range start=0 stop=5 scale=lin step-width=0.01 \$ Range 0 - 5; linear step of 0,01
 set-step-option element-content-in-wt%=yes \$ Composition in wt.%
 set-step-option temperature-in-celsius=yes \$ Temperature in Celsius
 set-step-option maximum-temperature-step=20 \$ Setting the max. T-step to 20
 step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series \$ Locking all unlocked series
 set-plot-option plot-id=. series rename series-index=-1 series-name=*_T\$C new-name=bcc_low \$ Renaming series: "*_T\$C" -
 --> "bcc_low"

\$----- Lower boundary of austenite -----\$
 set-temperature-celsius temperature=700 \$ Temperature 700C
 calculate-equilibrium
 search-phase-boundary phase-name=FCC_A1 temperature boundary search \$ Varying temperature for the phase

set-step-option type=phase-boundary \$ "Phase boundary" type
 set-step-option scheil-dependent-phase=FCC_A1 \$ Phase boundary of fcc phase field
 set-step-option element=C \$ Carbon content varied
 set-step-option range start=0 stop=5 scale=lin step-width=0.01 \$ Range 0 - 5; linear step of 0,01
 set-step-option element-content-in-wt%=yes \$ Composition in wt.%
 set-step-option temperature-in-celsius=yes \$ Temperature in Celsius
 set-step-option maximum-temperature-step=200 \$ Setting the max. T-step to 200
 step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series \$ Locking all unlocked series
 set-plot-option plot-id=. series rename series-index=-1 series-name=*_T\$C new-name=fcc2 \$ Renaming series: "*_T\$C" -
 -> "fcc2"

\$----- Graphite upper phase boundary -----\$
 set-temperature-celsius temperature=800 \$ Temperature 800C
 calculate-equilibrium
 search-phase-boundary phase-name=GRAPHITE temperature boundary search \$ Varying temperature for the phase

```

set-step-option type=phase-boundary          $ "Phase boundary" type
set-step-option scheil-dependent-phase=GRAPHITE    $ Phase boundary of graphite phase field
set-step-option element=C                      $ Carbon content varied
set-step-option range start=0 stop=5 scale=lin step-width=0.01    $ Range 0 - 5; linear step of 0,01
set-step-option element-content-in-wt%=yes        $ Composition in wt.%
set-step-option temperature-in-celsius=yes        $ Temperature in Celsius
set-step-option maximum-temperature-step=20      $ Setting the max. T-step to 20
step-equilibrium

set-plot-option plot-id=. series lock series-index=-1 series-name=T$C do-lock=yes    $ Locking the last series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T$C new-name=graphite $ Renaming series: "*_T$C"
--> "graphite"

$----- The finished diagram -----$
set-plot-option plot-id=. plot-title=Fe-C phase diagram    $ Plot title
set-plot-option plot-id=. y-axis-title=Temperature [C]      $ y-axis title
$ Scaling of y-axis starts from "400"
set-plot-option plot-id=. y-axis-scaling=400..

$$*****
                SAVING WORKSPACE
*****$$

$save-workspace "file-name"=Tutorial_8
save-workspace Tutorial_8

```

SCRIPT TUTORIAL 9

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for calculating pseudobinary phase diagrams according to Tutorial 9.
 The following contents will be covered:

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

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.

Database: mc_fe.tdb
 Author: P. Warczok
 Creation date: 10.11.2008
 Last update: 16.05.2019 (P. Warczok, Update for 6.02)
 This is a script for MatCalc version 6.02 (rel 1.003)

Known issues:

- "save-workspace file-name=Tutorial_9" is not working properly. Use "save-workspace Tutorial_9" instead.
- Dependent phase for the stepped calculation of "phase boundary" type can be defined either by "set-step-option scheil-dependent-phase=" or by "set-step-option T0-dependent-phase=", though this is not "Scheil" or "T0" calculation... Still, both of these seem to work fine in this role as well.

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module module-name=core \$ Use "core" module (MatCalc uses "core" module by default anyway)

new-workspace \$ creates a new workspace

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****
  
```

```

open-thermodynamic-database file-name=mc_fe.tdb          $ Thermodynamic database: mc_fe.tdb
select-elements elements=FE C NB VA                     $ Components: Fe, Nb, C
select-phases phases=LIQUID FCC_A1 BCC_A2 CEMENTITE     $ Phases: Liquid, fcc, bcc, cementite
read-thermodynamic-database

set-reference-element element=FE

enter-composition type=weight-percent composition=C=0,1 NB=0,3    $ Composition: 0.1 wt.% C, 0.3 wt.% Nb
Nb

set-automatic-startvalues
set-temperature-celsius temperature=1000                $ Temperature 1000C
calculate-equilibrium                                     $ Initial equilibrium
  
```

new-gui-window type-id=p1

\$ Phase diagram plot window

```

$$*****
FE-C PSEUDOBINARY WITH CONSTANT NB CONTENT
*****$$

```

```

$----- Upper boundary of delta-ferrite -----$
set-temperature-celsius temperature=1550          $ Temperature 1550C
calculate-equilibrium
search-phase-boundary phase-name=BCC_A2 temperature          $ Varying temperature for the phase
boundary search

```

```

set-step-option type=phase-boundary          $ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2          $ Phase boundary of bcc phase field
set-step-option element=C          $ Carbon content varied
set-step-option range start=0 stop=0,2 scale=lin step-width=0.0005          $ Range 0 - 0.2; linear step of 0,0005
set-step-option element-content-in-wt%=yes          $ Composition in wt.%
set-step-option temperature-in-celsius=yes          $ Temperature in Celsius
set-step-option maximum-temperature-step=20          $ Setting the ma(x). T-step to 20
step-equilibrium

```

```

set-plot-option plot-id=. series new buffer variable-name=T$c          $ Plotting the phase boundary
set-gui-window-property window-id=. duplicate-and-lock-plot-series          $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=bcc_high_1 $ Renaming series:
"*_T$c" --> "bcc_high_1"
set-plot-option plot-id=. grid which-grid=major enable-x-axis=yes          $ Switching on the major gridlines for x-
axis
set-plot-option plot-id=. grid which-grid=major enable-y-axis=yes          $ Switching on the major gridlines for y-
axis

```

```

$----- Lower boundary of liquid -----$
set-temperature-celsius temperature=1450          $ Temperature 1450C
calculate-equilibrium
search-phase-boundary phase-name=LIQUID temperature          $ Varying temperature for the phase
boundary search

```

```

set-step-option type=phase-boundary          $ "Phase boundary" type
set-step-option scheil-dependent-phase=LIQUID          $ Phase boundary of liquid phase field
set-step-option element=C          $ Carbon content varied
set-step-option range start=0 stop=0,2 scale=lin step-width=0.0005          $ Range 0 - 0.2; linear step of 0,0005
set-step-option element-content-in-wt%=yes          $ Composition in wt.%
set-step-option temperature-in-celsius=yes          $ Temperature in Celsius
set-step-option maximum-temperature-step=20          $ Setting the ma(x). T-step to 20
step-equilibrium

```

```

set-gui-window-property window-id=. duplicate-and-lock-plot-series          $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=liquid $ Renaming series: "*_T$c" -
-> "liquid"

```

```

$----- Upper boundary of austenite -----$
set-temperature-celsius temperature=1500          $ Temperature 1500C
calculate-equilibrium
search-phase-boundary phase-name=FCC_A1 temperature          $ Varying temperature for the phase
boundary search

```

```

set-step-option type=phase-boundary          $ "Phase boundary" type
set-step-option scheil-dependent-phase=FCC_A1          $ Phase boundary of fcc phase field
set-step-option element=C          $ Carbon content varied
set-step-option range start=0 stop=0,2 scale=lin step-width=0.0005          $ Range 0 - 0.2; linear step of 0,0005
set-step-option element-content-in-wt%=yes          $ Composition in wt.%

```

Appendix A

```

set-step-option temperature-in-celsius=yes                $ Temperature in Celsius
set-step-option maximum-temperature-step=20              $ Setting the ma(x). T-step to 20
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series    $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=fcc_1    $ Renaming series: "*_T$C" -
-> "fcc_1"

$----- Lower boundary of delta-ferrite -----$
set-temperature-celsius temperature=1450                  $ Temperature 1450C
calculate-equilibrium
search-phase-boundary phase-name=BCC_A2 temperature      $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                      $ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2            $ Phase boundary of bcc phase field
set-step-option element=C                                $ Carbon content varied
set-step-option range start=0 stop=0,2 scale=lin step-width=0.0005    $ Range 0 - 0,2; linear step of 0,0005
set-step-option element-content-in-wt%=yes               $ Composition in wt.%
set-step-option temperature-in-celsius=yes               $ Temperature in Celsius
set-step-option maximum-temperature-step=20              $ Setting the ma(x). T-step to 20
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series    $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=bcc_high_2 $ Renaming series:
"*_T$C" --> "bcc_high_2"

$----- Boundary of NbC phase -----$
set-temperature-celsius temperature=1450                  $ Temperature 1450C
calculate-equilibrium
search-phase-boundary phase-name=FCC_A1#01 temperature   $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                      $ "Phase boundary" type
set-step-option scheil-dependent-phase=FCC_A1#01         $ Phase boundary of NbC phase field
set-step-option element=C                                $ Carbon content varied
set-step-option range start=0 stop=0,2 scale=lin step-width=0.0005    $ Range 0 - 0,2; linear step of 0,0005
set-step-option element-content-in-wt%=yes               $ Composition in wt.%
set-step-option temperature-in-celsius=yes               $ Temperature in Celsius
set-step-option maximum-temperature-step=100             $ Setting the ma(x). T-step to 100
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series    $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=NbC      $ Renaming series: "*_T$C" -
-> "NbC"
set-plot-option plot-id=. y-axis-scaling=500..           $ Scaling on the y-axis starts from 500

$----- Upper boundary of alpha-ferrite -----$
set-temperature-celsius temperature=900                  $ Temperature 900C
calculate-equilibrium
search-phase-boundary phase-name=BCC_A2 temperature      $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                      $ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2            $ Phase boundary of bcc phase field
set-step-option element=C                                $ Carbon content varied
set-step-option range start=0 stop=0,2 scale=lin step-width=0.0005    $ Range 0 - 0,2; linear step of 0,0005
set-step-option element-content-in-wt%=yes               $ Composition in wt.%
set-step-option temperature-in-celsius=yes               $ Temperature in Celsius
set-step-option maximum-temperature-step=20              $ Setting the ma(x). T-step to 20

```

step-equilibrium

```
set-gui-window-property window-id=. duplicate-and-lock-plot-series      $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=bcc_low  $ Renaming series:
"*_T$c" --> "bcc_low"
```

```
$----- Lower boundary of austenite -----$
set-temperature-celsius temperature=700      $ Temperature 700C
calculate-equilibrium
search-phase-boundary phase-name=FCC_A1 temperature      $ Varying temperature for the phase
boundary search
```

```
set-step-option type=phase-boundary      $ "Phase boundary" type
set-step-option scheil-dependent-phase=FCC_A1      $ Phase boundary of fcc phase field
set-step-option element=C      $ Carbon content varied
set-step-option range start=0 stop=0,2 scale=lin step-width=0.0005      $ Range 0 - 0,2; linear step of 0,0005
set-step-option element-content-in-wt%=yes      $ Composition in wt.%
set-step-option temperature-in-celsius=yes      $ Temperature in Celsius
set-step-option maximum-temperature-step=20      $ Setting the ma(x). T-step to 20
step-equilibrium
```

```
set-gui-window-property window-id=. duplicate-and-lock-plot-series      $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=fcc2      $ Renaming series: "*_T$c" --
> "fcc2"
```

```
$----- Cementite upper phase boundary -----$
set-temperature-celsius temperature=850      $ Temperature 800C
calculate-equilibrium
search-phase-boundary phase-name=CEMENTITE temperature      $ Varying temperature for the phase
boundary search
```

```
set-step-option type=phase-boundary      $ "Phase boundary" type
set-step-option scheil-dependent-phase=CEMENTITE      $ Phase boundary of cementite phase field
set-step-option element=C      $ Carbon content varied
set-step-option range start=0 stop=0,2 scale=lin step-width=0.0005      $ Range 0 - 0,2; linear step of 0,0005
set-step-option element-content-in-wt%=yes      $ Composition in wt.%
set-step-option temperature-in-celsius=yes      $ Temperature in Celsius
set-step-option maximum-temperature-step=20      $ Setting the ma(x). T-step to 20
step-equilibrium
```

```
set-plot-option plot-id=. series lock series-index=-1 series-name=T$c do-lock=yes      $ Locking the last series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=cementite  $ Renaming series:
"*_T$c" --> "cementite"
```

```
$----- The finished diagram -----$
set-plot-option plot-id=. plot-title=Fe-C pseudobinary for 0.3 wt.% Nb      $ Plot title
set-gui-window-property window-id=. default-x-axis-title=Carbon content [wt.%]      $ x-axis title
set-plot-option plot-id=. y-axis-title=Temperature [C]      $ y-axis title
set-plot-option plot-id=. legend-alignment=right      $ Legend on the right
```

```
$$*****
FE-NB PSEUDOBINARY WITH CONSTANT C CONTENT
*****$$
```

```
new-gui-window type-id=p1      $ The new phase diagram will be plotted in the new GUI-
window
```

```

$----- Upper boundary of delta-ferrite -----$
set-temperature-celsius temperature=1550          $ Temperature 1550C
calculate-equilibrium
search-phase-boundary phase-name=BCC_A2 temperature          $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                $ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2      $ Phase boundary of bcc phase field
set-step-option element=NB                        $ Niobium content varied
set-step-option range start=0 stop=1 scale=lin step-width=0.01 $ Range 0 - 1; linear step of 0,01
set-step-option element-content-in-wt%=yes         $ Composition in wt.%
set-step-option temperature-in-celsius=yes         $ Temperature in Celsius
set-step-option maximum-temperature-step=20        $ Setting the ma(x). T-step to 20
step-equilibrium

set-plot-option plot-id=. series new buffer variable-name=T$C $ Plotting the phase boundary
set-gui-window-property window-id=. duplicate-and-lock-plot-series $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$C new-name=bcc_high_1 $ Renaming series:
"*_T$C" -> "bcc_high_1"
set-plot-option plot-id=. grid which-grid=major enable-x-axis=yes $ Switching on the major gridlines for x-
axis
set-plot-option plot-id=. grid which-grid=major enable-y-axis=yes $ Switching on the major gridlines for y-
axis

$----- Lower boundary of liquid -----$
set-temperature-celsius temperature=1450          $ Temperature 1450C
calculate-equilibrium
search-phase-boundary phase-name=LIQUID temperature          $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                $ "Phase boundary" type
set-step-option scheil-dependent-phase=LIQUID      $ Phase boundary of liquid phase field
set-step-option element=NB                        $ Niobium content varied
set-step-option range start=0 stop=1 scale=lin step-width=0.01 $ Range 0 - 1; linear step of 0,01
set-step-option element-content-in-wt%=yes         $ Composition in wt.%
set-step-option temperature-in-celsius=yes         $ Temperature in Celsius
set-step-option maximum-temperature-step=20        $ Setting the ma(x). T-step to 20
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$C new-name=liquid $ Renaming series: "*_T$C" -
-> "liquid"

$----- Upper boundary of austenite -----$
set-temperature-celsius temperature=1500          $ Temperature 1500C
calculate-equilibrium
search-phase-boundary phase-name=FCC_A1 temperature          $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                $ "Phase boundary" type
set-step-option scheil-dependent-phase=FCC_A1      $ Phase boundary of fcc phase field
set-step-option element=NB                        $ Niobium content varied
set-step-option range start=0 stop=1 scale=lin step-width=0.01 $ Range 0 - 1; linear step of 0,01
set-step-option element-content-in-wt%=yes         $ Composition in wt.%
set-step-option temperature-in-celsius=yes         $ Temperature in Celsius
set-step-option maximum-temperature-step=20        $ Setting the ma(x). T-step to 20
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series $ Locking all unlocked series

```

```
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=fcc_1    $ Renaming series: "*_t$c" -
-> "fcc_1"
```

```
$----- Lower boundary of delta-ferrite -----$
set-temperature-celsius temperature=1450          $ Temperature 1450C
calculate-equilibrium
search-phase-boundary phase-name=BCC_A2 temperature          $ Varying temperature for the phase
boundary search
```

```
set-step-option type=phase-boundary              $ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2      $ Phase boundary of bcc phase field
set-step-option element=NB                        $ Niobium content varied
set-step-option range start=0 stop=1 scale=lin step-width=0.01    $ Range 0 - 1; linear step of 0,01
set-step-option element-content-in-wt%=yes         $ Composition in wt.%
set-step-option temperature-in-celsius=yes         $ Temperature in Celsius
set-step-option maximum-temperature-step=20       $ Setting the ma(x). T-step to 20
step-equilibrium
```

```
set-gui-window-property window-id=. duplicate-and-lock-plot-series    $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=bcc_high_2 $ Renaming series:
"*_t$c" --> "bcc_high_2"
```

```
$----- Upper boundary of alpha-ferrite -----$
set-temperature-celsius temperature=900          $ Temperature 900C
calculate-equilibrium
search-phase-boundary phase-name=BCC_A2 temperature          $ Varying temperature for the phase
boundary search
```

```
set-step-option type=phase-boundary              $ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2      $ Phase boundary of bcc phase field
set-step-option element=NB                        $ Niobium content varied
set-step-option range start=0 stop=1 scale=lin step-width=0.01    $ Range 0 - 1; linear step of 0,01
set-step-option element-content-in-wt%=yes         $ Composition in wt.%
set-step-option temperature-in-celsius=yes         $ Temperature in Celsius
set-step-option maximum-temperature-step=20       $ Setting the ma(x). T-step to 20
step-equilibrium
```

```
set-gui-window-property window-id=. duplicate-and-lock-plot-series    $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=bcc_low    $ Renaming series:
"*_t$c" --> "bcc_low"
```

```
$----- Lower boundary of austenite -----$
set-temperature-celsius temperature=700          $ Temperature 700C
calculate-equilibrium
search-phase-boundary phase-name=FCC_A1 temperature          $ Varying temperature for the phase
boundary search
```

```
set-step-option type=phase-boundary              $ "Phase boundary" type
set-step-option scheil-dependent-phase=FCC_A1      $ Phase boundary of fcc phase field
set-step-option element=NB                        $ Niobium content varied
set-step-option range start=0 stop=1 scale=lin step-width=0.01    $ Range 0 - 1; linear step of 0,01
set-step-option element-content-in-wt%=yes         $ Composition in wt.%
set-step-option temperature-in-celsius=yes         $ Temperature in Celsius
set-step-option maximum-temperature-step=20       $ Setting the ma(x). T-step to 20
step-equilibrium
```

```
set-gui-window-property window-id=. duplicate-and-lock-plot-series    $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=fcc2    $ Renaming series: "*_t$c" --
> "fcc2"
```



```

$----- Cementite upper phase boundary -----$
set-temperature-celsius temperature=800                $ Temperature 800C
calculate-equilibrium
search-phase-boundary phase-name=CEMENTITE temperature    $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                    $ "Phase boundary" type
set-step-option scheil-dependent-phase=CEMENTITE        $ Phase boundary of cementite phase field
set-step-option element=Nb                             $ Niobium content varied
set-step-option range start=0 stop=1 scale=lin step-width=0.01    $ Range 0 - 1; linear step of 0,01
set-step-option element-content-in-wt%=yes              $ Composition in wt.%
set-step-option temperature-in-celsius=yes              $ Temperature in Celsius
set-step-option maximum-temperature-step=200           $ Setting the ma(x). T-step to 200
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series    $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$C new-name=cementite $ Renaming series:
"*_t$C" --> "cementite"

$----- Boundary of NbC phase (1) -----$
set-temperature-celsius temperature=1000                $ Temperature 1000C
calculate-equilibrium
search-phase-boundary phase-name=FCC_A1#01 temperature    $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                    $ "Phase boundary" type
set-step-option scheil-dependent-phase=FCC_A1#01        $ Phase boundary of NbC phase field
set-step-option element=Nb                             $ Niobium content varied
set-step-option range start=0 stop=1 scale=lin step-width=0.001    $ Range 0 - 1; linear step of 0,001
set-step-option element-content-in-wt%=yes              $ Composition in wt.%
set-step-option temperature-in-celsius=yes              $ Temperature in Celsius
set-step-option maximum-temperature-step=2              $ Setting the ma(x). T-step to 2
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series    $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$C new-name=NbC_1    $ Renaming series: "*_t$C"
--> "NbC_1"

$----- Boundary of NbC phase (2) -----$
set-temperature-celsius temperature=500                $ Temperature 500C
calculate-equilibrium

$ Searching a phase boundary of NbC phase field varying Nb content at 500C
search-phase-boundary phase-name=fcc_a1#01 element-content element=nb temperature=500 temperature-in-c=yes

set-step-option type=phase-boundary                    $ "Phase boundary" type
set-step-option scheil-dependent-phase=FCC_A1#01        $ Phase boundary of NbC phase field
set-step-option element=Nb                             $ Niobium content varied
set-step-option range start=0 stop=1 scale=lin step-width=0.001    $ Range 0 - 1; linear step of 0,001
set-step-option element-content-in-wt%=yes              $ Composition in wt.%
set-step-option temperature-in-celsius=yes              $ Temperature in Celsius
set-step-option maximum-temperature-step=200           $ Setting the ma(x). T-step to 200
step-equilibrium

set-plot-option plot-id=. series lock series-index=-1 series-name=T$C do-lock=yes    $ Locking the last series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$C new-name=NbC_2    $ Renaming series: "*_t$C"
--> "NbC_2"

$----- The finished diagram -----$

```

```

set-plot-option plot-id=. plot-title=Fe-Nb pseudobinary for 0.1 wt.% C          $ Plot title
set-gui-window-property window-id=. default-x-axis-title=Nb content [wt.%]      $ x-axis title
set-plot-option plot-id=. y-axis-title=Temperature [C]                          $ y-axis title
set-plot-option plot-id=. y-axis-scaling=500..                                  $ Scaling on the y-axis starts from 500
set-plot-option plot-id=. legend-alignment=right                               $ Legend on the right

$$*****
                        NB-C PSEUDOBINARY WITH CONSTANT FE CONTENT
*****$$

new-gui-window type-id=p1                $ This new phase diagram will be also plotted in the new
GUI-window

set-reference-element element=NB          $ Niobium content will be varied (Iron content will be
kept fix)
$ Initial system composition in mole fractions: 0,996 Fe, 0,003 C
enter-composition type=mole-fraction composition=FE=0,996 C=0,003

$----- Upper boundary of delta-ferrite -----$
set-temperature-celsius temperature=1550          $ Temperature 1550C
calculate-equilibrium
search-phase-boundary phase-name=BCC_A2 temperature          $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary              $ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2      $ Phase boundary of bcc phase field
set-step-option element=C                          $ Carbon content varied
set-step-option range start=0 stop=0,004 scale=lin step-width=1e-5          $ Range 0 - 0.005; linear step of 0.00001
set-step-option element-content-in-wt%=no          $ Composition in mole fraction
set-step-option temperature-in-celsius=yes          $ Temperature in Celsius
set-step-option maximum-temperature-step=20        $ Setting the ma(x). T-step to 20
step-equilibrium

set-plot-option plot-id=. series new buffer variable-name=T$C          $ Plotting the phase boundary
set-gui-window-property window-id=. duplicate-and-lock-plot-series      $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=bcc_high_1 $ Renaming series:
"*_T$C" --> "bcc_high_1"
set-plot-option plot-id=. grid which-grid=major enable-x-axis=yes        $ Switching on the major gridlines for x-
axis
set-plot-option plot-id=. grid which-grid=major enable-y-axis=yes        $ Switching on the major gridlines for y-
axis

$----- Lower boundary of liquid -----$
set-temperature-celsius temperature=1450          $ Temperature 1450C
calculate-equilibrium
search-phase-boundary phase-name=LIQUID temperature          $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary              $ "Phase boundary" type
set-step-option scheil-dependent-phase=LIQUID      $ Phase boundary of liquid phase field
set-step-option element=C                          $ Carbon content varied
set-step-option range start=0 stop=0,004 scale=lin step-width=1e-5          $ Range 0 - 0.005; linear step of 0.00001
set-step-option element-content-in-wt%=no          $ Composition in mole fraction
set-step-option temperature-in-celsius=yes          $ Temperature in Celsius
set-step-option maximum-temperature-step=20        $ Setting the ma(x). T-step to 20
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series      $ Locking all unlocked series

```

```
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$C new-name=liquid    $ Renaming series: "*_T$C" -
-> "liquid"
```

```
$----- Upper boundary of austenite -----$
set-temperature-celsius temperature=1500          $ Temperature 1500C
calculate-equilibrium
search-phase-boundary phase-name=FCC_A1 temperature          $ Varying temperature for the phase
boundary search
```

```
set-step-option type=phase-boundary              $ "Phase boundary" type
set-step-option scheil-dependent-phase=FCC_A1      $ Phase boundary of fcc phase field
set-step-option element=C                        $ Carbon content varied
set-step-option range start=0 stop=0,004 scale=lin step-width=1e-5      $ Range 0 - 0.005; linear step of 0.00001
set-step-option element-content-in-wt%=no          $ Composition in mole fraction
set-step-option temperature-in-celsius=yes          $ Temperature in Celsius
set-step-option maximum-temperature-step=20        $ Setting the ma(x). T-step to 20
step-equilibrium
```

```
set-gui-window-property window-id=. duplicate-and-lock-plot-series          $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$C new-name=fcc_1    $ Renaming series: "*_T$C" -
-> "fcc_1"
```

```
$----- Lower boundary of delta-ferrite -----$
set-temperature-celsius temperature=1450          $ Temperature 1450C
calculate-equilibrium
search-phase-boundary phase-name=BCC_A2 temperature          $ Varying temperature for the phase
boundary search
```

```
set-step-option type=phase-boundary              $ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2      $ Phase boundary of bcc phase field
set-step-option element=C                        $ Carbon content varied
set-step-option range start=0 stop=0,004 scale=lin step-width=1e-5      $ Range 0 - 0.005; linear step of 0.00001
set-step-option element-content-in-wt%=no          $ Composition in mole fraction
set-step-option temperature-in-celsius=yes          $ Temperature in Celsius
set-step-option maximum-temperature-step=20        $ Setting the ma(x). T-step to 20
step-equilibrium
```

```
set-gui-window-property window-id=. duplicate-and-lock-plot-series          $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$C new-name=bcc_high_2 $ Renaming series:
"*_T$C" --> "bcc_high_2"
```

```
$----- Upper boundary of alpha-ferrite -----$
set-temperature-celsius temperature=900          $ Temperature 900C
calculate-equilibrium
search-phase-boundary phase-name=BCC_A2 temperature          $ Varying temperature for the phase
boundary search
```

```
set-step-option type=phase-boundary              $ "Phase boundary" type
set-step-option scheil-dependent-phase=BCC_A2      $ Phase boundary of bcc phase field
set-step-option element=C                        $ Carbon content varied
set-step-option range start=0 stop=0,00399 scale=lin step-width=1e-5      $ Range 0 - 0.00498; linear step of
0.00001
set-step-option element-content-in-wt%=no          $ Composition in mole fraction
set-step-option temperature-in-celsius=yes          $ Temperature in Celsius
set-step-option maximum-temperature-step=20        $ Setting the ma(x). T-step to 20
step-equilibrium
```

```
set-gui-window-property window-id=. duplicate-and-lock-plot-series          $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$C new-name=bcc_low    $ Renaming series:
"*_T$C" --> "bcc_low"
```

```

$----- Lower boundary of austenite -----$
set-temperature-celsius temperature=700                                $ Temperature 700C
calculate-equilibrium
search-phase-boundary phase-name=FCC_A1 temperature                    $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                                  $ "Phase boundary" type
set-step-option scheil-dependent-phase=FCC_A1                        $ Phase boundary of fcc phase field
set-step-option element=C                                           $ Carbon content varied
set-step-option range start=0 stop=0.00399 scale=lin step-width=1e-5 $ Range 0 - 0.00498; linear step of
0.00001
set-step-option element-content-in-wt%=no                            $ Composition in mole fraction
set-step-option temperature-in-celsius=yes                           $ Temperature in Celsius
set-step-option maximum-temperature-step=20                          $ Setting the ma(x). T-step to 20
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series    $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=fcc2 $ Renaming series: "*_T$c" --
> "fcc2"

$----- Cementite upper phase boundary -----$
set-temperature-celsius temperature=800                                $ Temperature 800C
calculate-equilibrium
search-phase-boundary phase-name=CEMENTITE temperature                $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                                  $ "Phase boundary" type
set-step-option scheil-dependent-phase=CEMENTITE                    $ Phase boundary of cementite phase field
set-step-option element=C                                           $ Carbon content varied
set-step-option range start=0 stop=0.004 scale=lin step-width=1e-5   $ Range 0 - 0.005; linear step of 0.00001
set-step-option element-content-in-wt%=no                            $ Composition in mole fraction
set-step-option temperature-in-celsius=yes                           $ Temperature in Celsius
set-step-option maximum-temperature-step=20                          $ Setting the ma(x). T-step to 20
step-equilibrium

set-gui-window-property window-id=. duplicate-and-lock-plot-series    $ Locking all unlocked series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=cementite $ Renaming series:
"*_T$c" --> "cementite"

$----- Boundary of NbC phase (1) -----$
set-temperature-celsius temperature=1000                                $ Temperature 1000C
calculate-equilibrium
search-phase-boundary phase-name=FCC_A1#01 temperature                $ Varying temperature for the phase
boundary search

set-step-option type=phase-boundary                                  $ "Phase boundary" type
set-step-option scheil-dependent-phase=FCC_A1#01                    $ Phase boundary of NbC phase field
set-step-option element=C                                           $ Carbon content varied
set-step-option range start=0 stop=0.00396 scale=lin step-width=1e-5 $ Range 0 - 0.00396; linear step of
0.00001
set-step-option element-content-in-wt%=no                            $ Composition in mole fraction
set-step-option temperature-in-celsius=yes                           $ Temperature in Celsius
set-step-option maximum-temperature-step=20                          $ Setting the ma(x). T-step to 200
step-equilibrium

set-plot-option plot-id=. series lock series-index=-1 series-name=T$c do-lock=yes $ Locking the last series
set-plot-option plot-id=. series rename series-index=-1 series-name=*_t$c new-name=NbC $ Renaming series: "*_T$c" -
-> "NbC"

```

```

$----- The finished diagram -----$
set-plot-option plot-id=. plot-title=Nb-C pseudobinary for 0.995 Fe (mole fraction)      $ Plot title
set-gui-window-property window-id=. default-x-axis-title=C content [mole fr.]          $ x-axis title
set-plot-option plot-id=. y-axis-title=Temperature [C]                                $ y-axis title
set-plot-option plot-id=. y-axis-scaling=500..                                         $ Scaling on the y-axis starts from 500
set-plot-option plot-id=. legend-alignment=right                                       $ Legend on the right

$$*****
      SAVING WORKSPACE
*****$$

$save-workspace "file-name"=Tutorial_9
save-workspace Tutorial_9

```

SCRIPT TUTORIAL 10

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for T0-temperature in Fe-Cr-C according to Tutorial 10.
 The following contents will be covered:

- T0-temperature calculation
- Martensite / Bainite transformation
- Variation of T0-temperature with carbon and chromium content
- Import and display of experimental data into plots

Database: mc_fe.tdb
 Author: P. Warczok
 Creation date: 10.11.2008
 Last update: 20.05.2019 (P. Warczok, Update for 6.02)
 This is a script for MatCalc version 6.02 (rel 1.003)

Known issues:

- "save-workspace "file-name"=Tutorial_10" is not working properly. --> Use "save-workspace Tutorial_10" instead.
- load-calc-state calc-state-name="Start austenite" is not working. --> Use load-calc-state "Start austenite" instead.

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module module-name=core \$ Use "core" module (MatCalc uses "core" module by default anyway)

new-workspace \$ creates a new workspace

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****
  
```

open-thermodynamic-database file-name=mc_fe.tdb \$ Thermodynamic database: mc_fe.tdb
 select-elements elements=FE C CR VA \$ Components: Fe, C, Cr
 select-phases phases=FCC_A1 BCC_A2 \$ Phases: fcc, bcc
 read-thermodynamic-database

set-reference-element element=FE
 enter-composition type=weight-percent composition=C=0,1 CR=1 \$ Composition: 0.1 wt.% C, 1 wt.% Cr

set-automatic-startvalues
 set-temperature-celsius temperature=800 \$ Temperature 800C
 calculate-equilibrium \$ Initial equilibrium

```

$$*****
***** CALCULATE THE T0-TEMPERATURE *****
*****
  
```

search-phase-boundary phase-name=BCC_A2 temperature \$ Varying temperature for the bcc phase boundary search

```
create-calc-state new-state-name="Start austenite"
```

```
$ Searching the T0-temperature with bcc_a2 as a target phase and fcc_a1 as a parent phase.
```

```
$ The composition of target phase is forced to the one of the parent phase.
```

```
$ The dfm-offset is switched to 0
```

```
search-phase-boundary phase-name=BCC_A2 t0-temperature parent-phase=fcc_a1 force-parent-composition-for-target-  
phase=yes dfm-offset=0
```

```
$$*****  
      EVALUATE T0-TEMPERATURE AS A FUNCTION OF CHROMIUM CONTENT  
*****$$
```

```
set-step-option type=T0-temperature          $ Selects the type of calculation: "T0-temperature"  
set-step-option element=cr                   $ Chromium content varied  
set-step-option range start=0 stop=10 scale=lin step-width=0,5      $ Range 0 - 10; linear step of 0,5  
set-step-option temperature-in-celsius=yes    $ Temperature in Celsius  
set-step-option element-content-in-wt%=yes    $ Composition in wt.%  
set-step-option T0-dependent-phase=BCC_A2     $ The T0-dependent phase is bcc  
set-step-option T0-parent-phase=FCC_A1       $ The T0-parent phase is fcc  
$ The force parent composition option is switched to yes  
set-step-option T0-force-parent-composition=yes  
step-equilibrium
```

```
new-gui-window type-id=p1  
set-plot-option plot-id=. series new buffer variable-name=T$C        $ Plotting the T0-temperature  
set-gui-window-property window-id=. default-x-axis-title=Cr content [wt.%] $ x-axis title  
set-plot-option plot-id=. y-axis-title=T<sub>0</sub>-temperature [C]    $ y-axis title  
set-plot-option plot-id=. legend-alignment=none                      $ No legend  
set-plot-option plot-id=. grid which-grid=major enable-x-axis=yes     $ Switching on the major gridlines for x-axis  
set-plot-option plot-id=. grid which-grid=major enable-y-axis=yes     $ Switching on the major gridlines for y-axis
```

```
$$*****  
      EVALUATE T0-TEMPERATURE AS A FUNCTION OF CARBON CONTENT  
*****$$
```

```
rename-current-buffer new-buffer-name=T0-chromium
```

```
create-calc-buffer new-buffer-name=T0-carbon
```

```
$load-calc-state calc-state-name="Start austenite"
```

```
load-calc-state "start austenite"          $ Loads the last calc-state - "start_austenite"
```

```
set-step-option type=T0-temperature          $ Selects the type of calculation: "T0-temperature"  
set-step-option element=C                   $ Carbon content varied  
set-step-option range start=0 stop=1 scale=lin step-width=0,05      $ Range 0 - 1; linear step of 0,05  
set-step-option temperature-in-celsius=yes    $ Temperature in Celsius  
set-step-option element-content-in-wt%=yes    $ Composition in wt.%  
set-step-option T0-dependent-phase=BCC_A2     $ The T0-dependent phase is bcc  
set-step-option T0-parent-phase=FCC_A1       $ The T0-parent phase is fcc  
$ The force parent composition option is switched to yes  
set-step-option T0-force-parent-composition=yes  
step-equilibrium
```

```
set-gui-window-property window-id=. buffer-name="T0-carbon"          $ "T0-carbon" buffer results are plotted  
set-gui-window-property window-id=. default-x-axis-title=C content [wt.%] $ x-axis title
```

```
$$*****  
      ADD SOME EXPERIMENTAL DATA ON MARTENSITE START TEMPERATURES  
*****$$
```

```
create-calc-buffer new-buffer-name="T0 with offset"
```

```
create-global-table new-table-name=Exp_data          $ Creating table
```

\$ This command imports the data from the text file
 \$ Specify the path, if the source data is not in the working directory
 \$import-global-table table-name=exp_data file-name=t0_exp_temperatures.txt

```
add-table-entry table-name=Exp_data x-value=0 y-value=540          $ Adding to the "Exp_data" table the pair "0",
"540"Exp_data
add-table-entry table-name=Exp_data x-value=0.086 y-value=510      $ Adding to the "Exp_data" table the pair "0.086",
"510"
add-table-entry table-name=Exp_data x-value=0.1936 y-value=475     $ etc...
add-table-entry table-name=Exp_data x-value=0.2409 y-value=480
add-table-entry table-name=Exp_data x-value=0.2495 y-value=470
add-table-entry table-name=Exp_data x-value=0.2581 y-value=440
add-table-entry table-name=Exp_data x-value=0.3011 y-value=430
add-table-entry table-name=Exp_data x-value=0.3226 y-value=410
add-table-entry table-name=Exp_data x-value=0.3871 y-value=410
add-table-entry table-name=Exp_data x-value=0.3871 y-value=400
add-table-entry table-name=Exp_data x-value=0.3871 y-value=395
add-table-entry table-name=Exp_data x-value=0.4560 y-value=405
add-table-entry table-name=Exp_data x-value=0.4947 y-value=355
add-table-entry table-name=Exp_data x-value=0.5054 y-value=375
add-table-entry table-name=Exp_data x-value=0.6022 y-value=330
add-table-entry table-name=Exp_data x-value=0.6022 y-value=320
add-table-entry table-name=Exp_data x-value=0.7097 y-value=280
add-table-entry table-name=Exp_data x-value=0.7312 y-value=280
add-table-entry table-name=Exp_data x-value=0.7743 y-value=265
add-table-entry table-name=Exp_data x-value=0.8173 y-value=240
add-table-entry table-name=Exp_data x-value=0.8603 y-value=225
```

\$ In the current plot ("."), new series with the table/experimental data from "Exp_data" table is plotted
 set-plot-option plot-id=. series new table-experimental-data table-name=Exp_data
 set-plot-option plot-id=. legend-alignment=right \$ Legend on the right
 set-gui-window-property window-id=. duplicate-and-lock-plot-series \$ Locking all unlocked series (applies only to
 buffer result)
 \$ Renaming series: no.0 --> "T₀ - dfm = 0 J/mol"
 set-plot-option plot-id=. series rename series-index=-1 series-name=*_T\$C new-name="T₀ - dfm = 0 J/mol"
 set-plot-option plot-id=. series rename series-index=1 new-name=Exp_data \$ Renaming series: no.1 --> "Exp_data"
 set-gui-window-property window-id=. buffer-name="T0 with offset" \$ "T0_with_offset" buffer results are plotted

```
$----- dfm offset = 1200 J/mol -----$
set-step-option type=T0-temperature          $ Selects the type of calculation: "T0-temperature"
set-step-option element=C                    $ Carbon content varied
set-step-option range start=0 stop=1 scale=lin step-width=0,05    $ Range 0 - 1; linear step of 0,05
set-step-option temperature-in-celsius=yes    $ Temperature in Celsius
set-step-option element-content-in-wt%=yes    $ Composition in wt.%
set-step-option T0-dependent-phase=BCC_A2    $ The T0-dependent phase is bcc
set-step-option T0-parent-phase=FCC_A1       $ The T0-parent phase is fcc
$ The force parent composition option is switched to yes
set-step-option T0-force-parent-composition=yes
set-step-option T0-dfm-offset=1200           $ Sets the T0-dfm-offset to 1200 J/mol
step-equilibrium
```

```
set-gui-window-property window-id=. duplicate-and-lock-plot-series    $ Locking all unlocked series (applies only to
buffer result)
$ Renaming series: no.0 --> "T<sub>0</sub> - dfm = 1200 J/mol"
set-plot-option plot-id=. series rename series-index=-1 series-name=*_T$C new-name="T<sub>0</sub> - dfm = 1200 J/mol"
```

```
$----- dfm offset = 1700 J/mol -----$
set-step-option type=T0-temperature          $ Selects the type of calculation: "T0-temperature"
```



```

set-step-option element=C                $ Carbon content varied
set-step-option range start=0 stop=1 scale=lin step-width=0,05    $ Range 0 - 1; linear step of 0,05
set-step-option temperature-in-celsius=yes    $ Temperature in Celsius
set-step-option element-content-in-wt%=yes    $ Composition in wt.%
set-step-option T0-dependent-phase=BCC_A2    $ The T0-dependent phase is bcc
set-step-option T0-parent-phase=FCC_A1    $ The T0-parent phase is fcc
$ The force parent composition option is switched to yes
set-step-option T0-force-parent-composition=yes
set-step-option T0-dfm-offset=1700    $ Sets the T0-dfm-offset to 1700 J/mol
step-equilibrium

set-plot-option plot-id=. series lock series-index=-1 series-name=T$C do-lock=yes $ Locking the last series
$ Renaming series: no.0 --> "T<sub>0</sub> - dfm = 1700 J/mol"
set-plot-option plot-id=. series rename series-index=-1 series-name=_T$C new-name="T<sub>0</sub> - dfm = 1700 J/mol"

$$*****
          SAVING WORKSPACE
*****$$

$ Save workspace as "Tutorial_10.mcw"
$save-workspace "file-name"=Tutorial_10
save-workspace Tutorial_10

```

SCRIPT TUTORIAL 11

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for simulation of solidification of 0.7C 3Mn steel according to Tutorial 11.
 The following contents will be covered:

- 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. 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.

Database: mc_sample_fe.tdb
 Author: P. Warczok
 Creation date: 10.11.2008
 This is a script for MatCalc version 5.44 (rel 0.008)
 Last update: 26.09.2011 (G. Stechauner, Update for 5.44)

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module core \$ Use "core" module (MatCalc uses "core" module by default anyway)

new-workspace \$ creates a new workspace

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$ verify correct MatCalc version (is accessible as internal variable)
if (matcalc_version<5440008)
  send-dialog-string "MatCalc version must be 5.44.0008 or higher to run this script. Stopping."
  stop_run_script $ stop script
endif
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****
  
```

```

open-thermodyn-database mc_fe.tdb          $ Thermodynamic database: mc_sample_fe2.tdb
select-elements FE C MN VA                $ Components: Fe, C, Mn
select-phases LIQUID FCC_A1 BCC_A2 CEMENTITE $ Phases: Liquid, fcc, bcc, cementite
read-thermodyn-database
  
```

```

set-reference-element FE
enter-composition WP C=0,7 MN=3           $ Composition: 0.7 wt.% C, 3 wt.% Mn
  
```

```

set-temperature-celsius 1600              $ Temperature 1600C
set-automatic-startvalues
  
```

calculate-equilibrium \$ Initial equilibrium

```
$$*****
CARRY OUT A SCHEIL CALCULATION
*****$$
```

search-phase-boundary T FCC_A1 \$ Varying temperature for the fcc phase boundary search

```
set-step-option Y S                      $ Selects the t[y]pe of calculation: "[S]cheil"
$ Defines the [r]ange of the calculation: from 1500 to 1000 with linear step of 10
set-step-option R 1500 1000 10
set-step-option O C Y                    $ Temperature in Celsius
set-step-option P LIQUID                $ The dependent [p]hase is liquid
set-step-option L 1e-6                  $ The minimum [l]iquid fraction is set to 1e-6
```

step-equilibrium

```
$----- Creating a plot -----$
new-gui-window p1
```

```
set-gui-window-property . X T $C              $ Temperature in Celsius on x-axis
set-plot-option . A X 1 T T [C]              $ x-axis title
set-plot-option . A X 1 S 1100..              $ Scaling on the y-axis starts from 1100
set-plot-option . A Y 1 T Liquid fraction      $ y-axis title
set-plot-option . L R                      $ Legend on the right
set-plot-option . G M X Y                  $ Switching on the major gridlines for x-axis
set-plot-option . G M Y Y                  $ Switching on the major gridlines for y-axis
set-plot-option . S N B F $LIQUID %s              $ Plotting the fraction of the liquid phase
```

rename-current-buffer Scheil

```
$$*****
ADD A SCHEIL CALCULATION WITH BACK-DIFFUSION OF CARBON
*****$$
```

create-calc-buffer Scheil_with_BD_of_C

```
set-step-option Y S                      $ Selects the t[y]pe of calculation: "[S]cheil"
$ Defines the [r]ange of the calculation: from 1500 to 1000 with linear step of 10
set-step-option R 1500 1000 10
set-step-option O C Y                    $ Temperature in Celsius
set-step-option P LIQUID                $ The dependent [p]hase is liquid
set-step-option L 1e-6                  $ The minimum [l]iquid fraction is set to 1e-6
$ In the [b]ack diffusion section, [c]arbon diffusion is allowed (set to [y]es)
set-step-option B C Y
```

step-equilibrium

```
set-gui-window-property . L                  $ Locking all unlocked series
set-plot-option . S M -1 *_F$LIQUID Scheil      $ Renaming series: "*_F$LIQUID" --> "Scheil"
$ In the [b]uffer section, the data from buffer "Scheil_with_BD_of_C" are chosen for the display
set-gui-window-property . B Scheil_with_BD_of_C
set-gui-window-property . L                  $ Locking all unlocked series
$ Renaming series: "*_F$LIQUID" --> "Scheil with BD of C"
set-plot-option . S M -1 *_F$LIQUID 'Scheil with BD of C'
```

```
$$*****
ADD THE EQUILIBRIUM SOLIDIFICATION PATH
*****$$
```

```
change-phase-status FCC_A1_S F S S      $ Suspending phase "FCC_A1_S"
change-phase-status BCC_A2_S F S S      $ Suspending phase "BCC_A2_S"
change-phase-status CEMENTITE_S F S S    $ Suspending phase "CEMENTITE_S"
```

```
create-calc-buffer Equilibrium
```

```
set-step-option Y T                      $ "Temperature" type
set-step-option R 1500 1350 L 5          $ Range 1500 - 1350; linear step of 5
set-step-option O C Y                    $ Temperature in Celsius
```

```
step-equilibrium
```

```
$ In the [b]uffer section, the data from buffer "Equilibrium" are chosen for the display
```

```
set-gui-window-property . B Equilibrium
```

```
set-plot-option . S L -1 F$LIQUID Y      $ Locking the series "F$LIQUID"
```

```
set-plot-option . S M -1 *_F$LIQUID Equilibrium $ Renaming series: " *_F$LIQUID" --> "Equilibrium"
```

```
$ In the [a]xis section for the [y]-axis no.[1], the scaling t[y]pe is set to [log]arithmic
```

```
set-plot-option . A Y 1 Y log
```

```
set-plot-option . A Y 1 S 0,01..         $ Scaling on the y-axis starts from 0.01
```

```
$$*****
      SAVING WORKSPACE
*****$$
```

```
save-workspace Tutorial_11
```

SCRIPT TUTORIAL 12

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for using the MatCalc console according to Tutorial 12.
 The following contents will be covered:

- 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

Database: mc_sample_fe.tdb

Author: P. Warczok

Creation date: 10.11.2008

This is a script for MatCalc version 5.44 (rel 0.008)

Last update: 26.09.2011 (G. Stechauner, Update for 5.44)

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module core \$ Use "core" module (MatCalc uses "core" module by default anyway)

new-workspace \$ creates a new workspace

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

\$ verify correct MatCalc version (is accessible as internal variable)

if (matcalc_version<5440008)

send-dialog-string "MatCalc version must be 5.44.0008 or higher to run this script. Stopping."

stop_run_script \$ stop script

endif

```

$$*****
***** BASICS *****
*****
  
```

help-workspace \$ Opens a list of available commands in workspace module

help-module core \$ Opens a list of available commands in mc_core

```

$$*****
***** EXAMPLE: CALCULATING AND EQUILIBRIUM USING THE COMMAND-LINE *****
*****
  
```

open-thermodyn-database mc_fe.tdb \$ Thermodynamic database: mc_sample_fe2.tdb

\$ Lists the contents of the thermodynamic ([e]quilibrium) database

list-database-contents E

select-elements C FE \$ Components: Fe, C

select-phases LIQUID BCC_A2 FCC_A1 CEMENTITE \$ Selects the liquid, bcc, fcc and cementite phases

read-thermodyn-database

Appendix A

enter-composition WP C=0,4 \$ Composition: 0.4 wt.% C

set-temperature-celsius 700 \$ Temperature 700C

set-automatic-startvalues

calculate-equilibrium \$ Initial equilibrium

\$\$*****

EVALUATING EXPRESSIONS

*****\$\$

\$----- Numerical expressions ----- \$

show-expression 4/5

show-expression pi

show-expression 4/5*3

show-expression 4/(5*3)

show-expression 4+4*2

show-expression (4+4)*2

\$----- Expressions in x ----- \$

show-expression 3*x

set-function-expression function1 3*x \$ Defining function1

set-function-expression function2 x**2 \$ Defining function2

set-function-expression function3 x^2 \$ Defining function3

new-gui-window p1

\$\$ For the current plot[,], in [s]eries section, [n]ew series with the [f]unction/expression
result for "function1" is plotted in the range of -10 - 10 \$\$

set-plot-option . S N F function1 -10..10

\$ Plotting the result for "function2" is plotted in the range of -10 - 10

set-plot-option 1 S N F function2 -10..10

\$ Plotting the result for "function3" is plotted in the range of -10 - 10

set-plot-option 1 S N F function3 -10..10

\$\$*****

EXPRESSIONS USING MATCALC VARIABLES

*****\$\$

set-function-expression function4 F\$BCC_A2*X\$BCC_A2\$C \$ Defining function4

set-function-expression function5 F\$CEMENTITE*X\$CEMENTITE\$C \$ Defining function5

show-expression function4

show-expression function5

show-expression function4+function5

show-expression X\$C-(function4+function5)

\$\$*****

SAVING WORKSPACE

*****\$\$

save-workspace Tutorial_12

SCRIPT TUTORIAL 13

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for introduction to scripting (1: Equilibrium calculations) according to Tutorial 13.
 The following contents will be covered:

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

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.

Database: mc_sample_fe.tdb
 Author: P. Warczok
 Creation date: 10.11.2008
 This is a script for MatCalc version 5.44 (rel 0.008)
 Last update: 26.09.2011 (G. Stechauner, Update for 5.44)

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module core \$ Use "core" module (MatCalc uses "core" module by default anyway)

new-workspace \$ creates a new workspace

```

@ echo n    $ Hides command name in console
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.
echo y      $ Shows command name in console
  
```

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$ verify correct MatCalc version (is accessible as internal variable)
if (matcalc_version<5440008)
  send-dialog-string "MatCalc version must be 5.44.0008 or higher to run this script. Stopping."
  stop-run-script $ stop script
endif
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****
  
```

```

open-thermodyn-database mc_fe.tdb      $ Thermodynamic database: mc_sample_fe.tdb
select-elements c fe                  $ Components: Fe, Nb, C
select-phases liq bcc_a2 fcc cem      $ Phases: Liquid, bcc, fcc, cementite
  
```

read-thermodyn-database

set-reference-element FE

enter-composition wp c=0.4 \$ Composition: 0.4 wt.% C

set-temperature-celsius 700

\$ Temperature 700C

set-automatic-startvalues

calculate-equilibrium \$ Initial equilibrium

\$\$*****

GRAPHICAL OUTPUT

*****\$\$

set-step-option r 400 1600 L 25

step-equilibrium

new-gui-window p1

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

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

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

set-plot-option . s n b f\$liquid

set-plot-option . s m -1 f\$liquid Liquid

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 Fe₃</sub>C

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.

create-new-plot x .

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 Fe₃</sub>C

\$\$*****

SAVING WORKSPACE

*****\$\$

save-workspace Tutorial_13

SCRIPT TUTORIAL 14

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for introduction to precipitation calculations according to Tutorial 14.
 The following contents will be covered:

- 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

Database: mc_sample_fe.tdb
 Author: P. Warczok
 Creation date: 18.11.2008
 This is a script for MatCalc version 5.44 (rel 0.008)
 Last update: 23.05.2018 (P. Warczok, Update for 6.01)

```

*****
***** SETUP INFORMATION *****
*****
  
```

\$ Use "core" module (MatCalc uses "core" module by default anyway)
 use-module module-name=core

new-workspace \$ creates a new workspace

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$ verify correct MatCalc version (is accessible as internal variable)
if (matcalc_version<6011000)
  send-dialog-string "MatCalc version must be 6.01.1000 or higher to run this script. Stopping."
  stop-run-script $ stop script
endif
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****
  
```

```

open-thermodynamic-database file-name=mc_fe.tdb      $ Thermodynamic database: mc_sample_fe.tdb
select-elements elements=FE C VA                    $ Components: Fe, C
select-phases phases=BCC_A2 CEMENTITE              $ Phases: bcc, cementite
read-thermodynamic-database
  
```

```

set-reference-element element=FE
enter-composition type=weight-percent composition= C=0,2    $ Composition: 0.2 wt.% C
  
```

```

$----- Precipitation domain -----$
create-precipitation-domain new-domain-name=Ferrite      $ Creates precipitation domain "Ferrite"
  
```

```

$ "Ferrite" is defined as a matrix phase with bcc structure
set-precipitation-parameter precipitate-or-domain-name=Ferrite thermodynamic-matrix-phase=BCC_A2
  
```

```

$----- Precipitate phase -----$
create-new-phase CEMENTITE precipitate          $ Cementite is defined as a precipitate phase
$ Initializes the precipitate phase cementite_p0 with 250 classes
set-precipitation-parameter CEMENTITE_P0 number-of-size-classes=250
$ Dislocations are set as nucleation sites
set-precipitation-parameter CEMENTITE_P0 nucleation-sites=dislocations

$----- Loading mobility data -----$
read-mobility-database file-name=mc_fe.ddb        $ Mobility (diffusion) database: mc_sample_fe.ddb

$----- Creating plots for the output -----$
new-gui-window type-id=p1
set-gui-window-property window-id=. default-x-axis-for-all-plots=yes  $ Default x-axis
set-gui-window-property window-id=. default-x-axis-title=Time [h]      $ x-axis title
set-gui-window-property window-id=. default-x-axis-type=log            $ Logarithmic scale on x-axis
set-gui-window-property window-id=. default-x-axis-scaling=1e-12..     $ Scaling starts from 1e-12
set-gui-window-property window-id=. default-x-axis-factor=1/3600       $ Multiplication [f]actor for x-axis

set-plot-option plot-id=. plot-title=Phase fraction of cementite precipitate  $ Plot title
set-plot-option plot-id=. y-axis-title=Phase fraction                      $ y-axis title
set-plot-option plot-id=. legend-alignment=none                          $ None legend box
set-plot-option plot-id=. series new buffer variable-name=F$CEMENTITE_P0    $ Plotting the fraction of cementite
precipitate phase

new-gui-window type-id=p5          $ Creating a window with histogram
set-gui-window-property window-id=. default-x-axis-for-all-plots=no        $ Do not use default x-axis
$ Plot precipitate distribution of "cementite_p0" phase
set-plot-option plot-id=. series new precipitate-distribution phase-name=CEMENTITE_P0
$ Divide the size range in histogram into 20 classes
set-plot-option plot-id=. number-of-size-classes=20
set-plot-option plot-id=. plot-title=Cementite precipitate distribution      $ Plot title
set-plot-option plot-id=. x-axis-title=Precipitate radius [nm]              $ x-axis title
set-plot-option plot-id=. x-axis-factor=1e9                                $ Multiplication factor for x-axis
set-plot-option plot-id=. y-axis-title=Number of precipitates              $ y-axis title
set-plot-option plot-id=. legend-alignment=none                          $ None legend box

$$*****
THE CALCULATION
*****$$

$ Numerical limit for nucleation density is set to 1,05 to obtain 250 classes in the simulation
set-simulation-parameter nucleation-density-increase-factor=1,05

set-temperature-celsius temperature=600          $ Temperature 600C
set-automatic-startvalues
calculate-equilibrium                            $ Initial equilibrium

set-simulation-parameter end-time=3,6e3          $ Simulation end time is set to 3600 seconds (1 hour)

$ Simulation is performed at the constant temperature of 600°C
set-simulation-parameter isothermal-temperature=600
set-simulation-parameter temperature-in-C=yes     $ Temperature value expressed in degree Celsius

start-precipitate-simulation                    $ Starts kinetic simulation

$$*****
INTERPRETING THE RESULTS
*****$$

```

```

create-new-plot plot-type=xy-plot attach-to-window=2
set-plot-option plot-id=. plot-title=Number of precipitates          $ Plot title
set-plot-option plot-id=. y-axis-title=Number of precipitates [ $10^{20}$  m-3] $ y-axis title
set-plot-option plot-id=. x-axis-factor=1e-20                      $ Multiplication factor for y-axis
set-plot-option plot-id=. legend-alignment=none                    $ No legend
$ Plotting the number of particles of cementite precipitate
set-plot-option plot-id=. series new buffer variable-name=NUM_PART$CEMENTITE_PO

create-new-plot plot-type=xy-plot attach-to-window=2
set-plot-option plot-id=. plot-title=Nucleation rate                $ Plot title
set-plot-option plot-id=. y-axis-title=Nucleation rate [ $10^{26}$  m-3s-1] $ y-axis title
set-plot-option plot-id=. x-axis-factor=1e-26                      $ Multiplication factor for y-axis
set-plot-option plot-id=. legend-alignment=none                    $ No legend
$ Plotting the nucleation rate of cementite precipitate
set-plot-option plot-id=. series new buffer variable-name=NUCL_RATE$CEMENTITE_PO

create-new-plot plot-type=xy-plot attach-to-window=2
set-plot-option plot-id=. plot-title=Precipitate radius            $ Plot title
set-plot-option plot-id=. y-axis-title=Precipitate radius [ $10^{-6}$  m] $ y-axis title
set-plot-option plot-id=. y-axis-type=log                          $ Logarithmic scale on y-axis
set-plot-option plot-id=. x-axis-factor=1e6                        $ Multiplication factor for y-axis
set-plot-option plot-id=. legend-alignment=bottom                  $ Legend on the bottom
set-plot-option plot-id=. series new buffer variable-name=R_MEAN$CEMENTITE_PO $ Plotting mean radius of cementite
precipitate
set-plot-option plot-id=. series new buffer variable-name=R_CRIT$CEMENTITE_PO $ Plotting critical radius of cementite
precipitate
set-plot-option plot-id=. series new buffer variable-name=R_MIN$CEMENTITE_PO $ Plotting minimal radius of cementite
precipitate
set-plot-option plot-id=. series new buffer variable-name=R_MAX$CEMENTITE_PO $ Plotting maximal radius of cementite
precipitate
set-plot-option plot-id=. series rename series-index=0 new-name=Mean $ Renaming series no. 0 to "Mean"
set-plot-option plot-id=. series rename series-index=1 new-name=Critical $ Renaming series no. 1 to "Critical"
set-plot-option plot-id=. series rename series-index=2 new-name=Min $ Renaming series no. 2 to "Min"
set-plot-option plot-id=. series rename series-index=3 new-name=Max $ Renaming series no. 3 to "Max"

set-plot-option plot-id=1 grid which-grid=major enable-x-axis=yes $ Switching on the major gridlines for x-axis for
plot no. 1
set-plot-option plot-id=1 grid which-grid=major enable-y-axis=yes $ Switching on the major gridlines for y-axis for
plot no. 1
set-plot-option plot-id=3 grid which-grid=major enable-x-axis=yes $ Switching on the major gridlines for x-axis for
plot no. 3
set-plot-option plot-id=3 grid which-grid=major enable-y-axis=yes $ Switching on the major gridlines for y-axis for
plot no. 3
set-plot-option plot-id=4 grid which-grid=major enable-x-axis=yes $ Switching on the major gridlines for x-axis for
plot no. 4
set-plot-option plot-id=4 grid which-grid=major enable-y-axis=yes $ Switching on the major gridlines for y-axis for
plot no. 4
set-plot-option plot-id=5 grid which-grid=major enable-x-axis=yes $ Switching on the major gridlines for x-axis for
plot no. 5
set-plot-option plot-id=5 grid which-grid=major enable-y-axis=yes $ Switching on the major gridlines for y-axis for
plot no. 5
set-gui-window-property window-id=. number-of-plot-columns=2      $ Arranging plots in the columns with the
[n]umber of columns of "2"

create-new-plot plot-type=precipitate-distribution attach-to-window=3 $ New histogram plot
$ Plot precipitate distribution of "cementite_p0" phase
set-plot-option plot-id=. series new precipitate-distribution phase-name=CEMENTITE_PO
set-plot-option plot-id=. number-of-size-classes=20                $ Divide the size range in histogram into 20 classes
$ Setting histogram frequency scaling to density
set-plot-option plot-id=. histogram scale-frequency=density
$ Setting histogram x-axis to show scaled radius
set-plot-option plot-id=. histogram scale-radius=yes

```

```
set-plot-option plot-id=. plot-title=Scaled cementite precipitate size distribution $ Plot title
set-plot-option plot-id=. x-axis-title=Scaled radius $ x-axis title
set-plot-option plot-id=. y-axis-title=Scaled number $ y-axis title
set-plot-option plot-id=. x-axis-scaling=0..1,499 $ x-axis scaling in range 0 - 1.499
set-plot-option plot-id=. legend-alignment=bottom $ Legend on the bottom

$ Definition of "lsw" function
set-function-expression function=lsw expression=x^2*(3/(3+x))^(7/3)*((3/2)/(3/2-x))^(11/3)*exp(-x/(3/2-x))*4/9
$ Plotting the "lsw" function in the range 0 - 1.499
set-plot-option plot-id=. series new functional-expression expression-in-variable-x=lsw definition-range=0..1,499
```

```
$$*****
                        SAVING WORKSPACE
*****$$
```

```
save-workspace Tutorial_14
```

SCRIPT TUTORIAL 15

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for effect of microstructure and conditions (Part 1) according to Tutorial 15.
 The following contents will be covered:

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

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 600C. 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 (Fe₃C) phase, and Tutorial 16 will consider the interaction between this and the more stable phase M₂₃C₆.

Database: mc_sample_fe.tdb
 Author: P. Warczok
 Creation date: 10.11.2008
 This is a script for MatCalc version 5.44 (rel 0.008)
 Last update: 26.09.2011 (G. Stechauner, Update for 5.44)

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module core \$ Use "core" module (MatCalc uses "core" module by default anyway)

new-workspace \$ creates a new workspace

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$ verify correct MatCalc version (is accessible as internal variable)
if (matcalc_version<5440008)
  send-dialog-string "MatCalc version must be 5.44.0008 or higher to run this script. Stopping."
  stop-run-script $ stop script
endif
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****
  
```

```

open-thermodyn-database mc_fe.tdb          $ Thermodynamic database: mc_sample_fe2.tdb
select-elements FE C CR VA                 $ Components: Fe, C, Cr
select-phases BCC_A2 CEMENTITE M23C6       $ Phases: bcc, cementite, M23C6
read-thermodyn-database
  
```

```

set-reference-element FE
enter-composition WP C=0,1 CR=10           $ Composition: 0.1 wt.% C, 10 wt.% Cr
  
```

```
set-temperature-celsius 600          $ Temperature 600C
set-automatic-startvalues
calculate-equilibrium                $ Initial equilibrium
```

```
change-phase-status M23C6 F S S      $ M23C6 phase suspended
calculate-equilibrium
change-phase-status M23C6 F S C      $ M23C6 phase activated
calculate-equilibrium
```

```
$$*****
NUCLEATION MODEL FOR CEMENTITE
*****$$
```

```
$----- Setting up the simulation -----$
create-new-phase CEMENTITE P          $ Cementite is defined as a precipitate phase
$ Initializes the precipitate phase cementite_p0 with 25 [c]lasses
set-precipitation-parameter CEMENTITE_P0 C 25
$ In the [n]ucleation section, the nucleation [s]ites are set to [d]islocations
set-precipitation-parameter CEMENTITE_P0 N S D
$ In the [n]ucleation section, the nucleus [c]omposition is set as [p]ara-composition
set-precipitation-parameter CEMENTITE_P0 N C P
$set-precipitation-parameter CEMENTITE_P0 special ipdcf-radius-exponent=0,5

create-precipitation-domain ferrite    $ Creates precipitation domain "ferrite"
$ "Ferrite" is defined as a matrix phase with bcc structure
set-precipitation-parameter ferrite X BCC_A2

read-mobility-database mc_fe.ddb      $ Mobility (diffusion) database: mc_sample_fe.ddb
```

```
$----- Graphical display of results -----$
new-gui-window p1
set-gui-window-property . S U Y        $ Use default x-axis
set-gui-window-property . S T Time [h]  $ Default x-axis title
set-gui-window-property . S Y log       $ Logarithmic scale on default x-axis
set-gui-window-property . S S 1e-10..  $ Scaling limit for the default x-axis
set-gui-window-property . S F 1/3600    $ Multiplication factor for the default x-axis

set-plot-option . S N B F$CEMENTITE_P0 %s    $ Plotting the fraction of cementite phase
set-plot-option . A Y 1 T f<sub>CEM</sub>    $ y-axis title

create-new-plot X .
$ Plotting the chromium content in the cementite precipitate
set-plot-option . S N B X$CEMENTITE_P0$CR %s
$ Plotting the chromium content in the cementite precipitate nucleus
set-plot-option . S N B X_NUCL$CEMENTITE_P0$CR %s
set-plot-option . A Y 1 T x<sub>Cr</sub>    $ y-axis title

create-new-plot X .
set-plot-option . S N B X$BCC_A2$C %s        $ Plotting the carbon content in the bcc phase
set-plot-option . A Y 1 T x<sub>BCC_A2, C</sub> $ y-axis title

create-new-plot X .
$ Plotting the number of particles of cementite precipitate
set-plot-option . S N B NUM_PREC$CEMENTITE_P0 %s
$ y-axis title
set-plot-option . A Y 1 T N<sub>ppt</sub> [m<sup>-3</sup>]

create-new-plot X .
set-plot-option . S N B R_MEAN$CEMENTITE_P0 %s $ Plotting the mean radius of cementite precipitate
set-plot-option . A Y 1 T R<sub>mean</sub> [m] $ y-axis title
set-plot-option . A Y 1 Y log              $ Logarithmic scale on y-axis
```

```

set-plot-option 1 G M X Y      $ Switching on the major gridlines for x-axis for plot no. 1
set-plot-option 1 G M Y Y      $ Switching on the major gridlines for y-axis for plot no. 1
set-plot-option 2 G M X Y      $ Switching on the major gridlines for x-axis for plot no. 2
set-plot-option 2 G M Y Y      $ Switching on the major gridlines for y-axis for plot no. 2
set-plot-option 3 G M X Y      $ Switching on the major gridlines for x-axis for plot no. 3
set-plot-option 3 G M Y Y      $ Switching on the major gridlines for y-axis for plot no. 3
set-plot-option 4 G M X Y      $ Switching on the major gridlines for x-axis for plot no. 4
set-plot-option 4 G M Y Y      $ Switching on the major gridlines for y-axis for plot no. 4
set-plot-option 5 G M X Y      $ Switching on the major gridlines for x-axis for plot no. 5
set-plot-option 5 G M Y Y      $ Switching on the major gridlines for y-axis for plot no. 5
$ Arranging plots in the columns with the [n]umber of columns of "2"
set-gui-window-property . N 2

```

```

save-workspace Tutorial_15_setup

```

```

$$*****
                        CALCULATION
*****$$

```

```

$----- Para-equilibrium -----$
set-simulation-parameter E 3,6e13      $ Simulation end tim[e] is set to 3.6e13 seconds

```

```

$ In [t]emperature section, [i]sothermal option is chosen with 600
set-simulation-parameter T I 600
set-simulation-parameter P Y           $ Tem[p]erature in Celsius
set-simulation-parameter convergence-control numerical-limits-precipitation minimum-dfm-for-matrix-compensation=0,25
start-precipitate-simulation           $ Starts kinetic simulation

```

```

set-gui-window-property . L           $ Locking all unlocked series
set-plot-option 1 S M 0 Para          $ Renaming series in plot #1: #0 --> "Para"
$ Renaming series in plot #2: #0 --> "X<sub>CEM</sub>, Para"
set-plot-option 2 S M 0 'X<sub>CEM</sub>, Para'
$ Renaming series in plot #2: #1 --> "X<sub>NUCL,CEM</sub>, Para"
set-plot-option 2 S M 1 'X<sub>NUCL,CEM</sub>, Para'
set-plot-option 3 S M 0 Para          $ Renaming series in plot #3: #0 --> "Para"
set-plot-option 4 S M 0 Para          $ Renaming series in plot #4: #0 --> "Para"
set-plot-option 5 S M 0 Para          $ Renaming series in plot #5: #0 --> "Para"

```

```

$----- Ortho-equilibrium -----$
$ In the [n]ucleation section, the nucleus [c]omposition is set as [o]rtho-composition
set-precipitation-parameter CEMENTITE_P0 N C O
start-precipitate-simulation

```

```

set-plot-option 1 S M 1 Ortho         $ Renaming series in plot #1: #1 --> "Ortho"
$ Renaming series in plot #2: #2 --> "X<sub>CEM</sub>, Ortho"
set-plot-option 2 S M 2 'X<sub>CEM</sub>, Ortho'
$ Renaming series in plot #2: #3 --> "X<sub>NUCL,CEM</sub>, Ortho"
set-plot-option 2 S M 3 'X<sub>NUCL,CEM</sub>, Ortho'
set-plot-option 3 S M 1 Ortho         $ Renaming series in plot #3: #1 --> "Ortho"
set-plot-option 4 S M 1 Ortho         $ Renaming series in plot #4: #1 --> "Ortho"
set-plot-option 5 S M 1 Ortho         $ Renaming series in plot #5: #1 --> "Ortho"

```

```

$$*****
                        DIFFUSIVITY IN PRECIPITATES
*****$$

```

```

set-gui-window-property . L           $ Locking all unlocked series
$ Renaming series in plot #1: #2 --> "Para, faster diffusion in ppt"
set-plot-option 1 S M 2 'Para, faster diffusion in ppt'

```

```
$ Renaming series in plot #2: #4 --> "X<sub>CEM</sub>, Para, faster diffusion in ppt"
set-plot-option 2 S M 4 'X<sub>CEM</sub>, Para, faster diffusion in ppt'
$ Renaming series in plot #2: #5 --> "X<sub>NUCL,CEM</sub>, Para, faster diffusion in ppt"
set-plot-option 2 S M 5 'X<sub>NUCL,CEM</sub>, Para, faster diffusion in ppt'
$ Renaming series in plot #3: #2 --> "Para, faster diffusion in ppt"
set-plot-option 3 S M 2 'Para, faster diffusion in ppt'
$ Renaming series in plot #4: #2 --> "Para, faster diffusion in ppt"
set-plot-option 4 S M 2 'Para, faster diffusion in ppt'
$ Renaming series in plot #5: #2 --> "Para, faster diffusion in ppt"
set-plot-option 5 S M 2 'Para, faster diffusion in ppt'
```

```
$ Para-composition for cementite precipitate nucleus
set-precipitation-parameter CEMENTITE_PO N C P
$ [S]pecial options, [d]iffusion in prec. is calculated from matrix diffusion with [r]atio of 0.25
set-precipitation-parameter CEMENTITE_PO S D R 0,25
start-precipitate-simulation
```

```
$$*****
MICROSTRUCTURAL PARAMETERS AND NUCLEATION SITES
*****$$
```

```
set-plot-option 1 S R -1 Ortho      $ Removing "Ortho" series in plot #1
$ Removing "X<sub>CEM</sub>, Ortho" series in plot #2
set-plot-option 2 S R -1 'X<sub>CEM</sub>, Ortho'
$ Removing "X<sub>NUCL,CEM</sub>, Ortho" series in plot #2
set-plot-option 2 S R -1 'X<sub>NUCL,CEM</sub>, Ortho'
set-plot-option 3 S R -1 Ortho      $ Removing "Ortho" series in plot #3
set-plot-option 4 S R -1 Ortho      $ Removing "Ortho" series in plot #4
set-plot-option 5 S R -1 Ortho      $ Removing "Ortho" series in plot #5
```

```
$ Renaming series in plot #1: #0 --> "10<sup>-12</sup>m<sup>2</sup>"
set-plot-option 1 S M 0 10<sup>-12</sup>m<sup>2</sup>
$ Renaming series in plot #2: #0 --> "10<sup>-12</sup>m<sup>2</sup>"
set-plot-option 2 S M 0 10<sup>-12</sup>m<sup>2</sup>
$ Renaming series in plot #2: #1 --> "nucl_10<sup>-12</sup>m<sup>2</sup>"
set-plot-option 2 S M 1 nucl_10<sup>-12</sup>m<sup>2</sup>
$ Renaming series in plot #3: #0 --> "10<sup>-12</sup>m<sup>2</sup>"
set-plot-option 3 S M 0 10<sup>-12</sup>m<sup>2</sup>
$ Renaming series in plot #4: #0 --> "10<sup>-12</sup>m<sup>2</sup>"
set-plot-option 4 S M 0 10<sup>-12</sup>m<sup>2</sup>
$ Renaming series in plot #5: #0 --> "10<sup>-12</sup>m<sup>2</sup>"
set-plot-option 5 S M 0 10<sup>-12</sup>m<sup>2</sup>
```

```
$----- Dislocation density 1e14 -----$
$ Renaming series in plot #1: #1 --> "10<sup>-14</sup>m<sup>2</sup>"
set-plot-option 1 S M 1 10<sup>-14</sup>m<sup>2</sup>
$ Renaming series in plot #2: #2 --> "10<sup>-14</sup>m<sup>2</sup>"
set-plot-option 2 S M 2 10<sup>-14</sup>m<sup>2</sup>
$ Renaming series in plot #2: #3 --> "nucl_10<sup>-14</sup>m<sup>2</sup>"
set-plot-option 2 S M 3 nucl_10<sup>-14</sup>m<sup>2</sup>
$ Renaming series in plot #3: #1 --> "10<sup>-14</sup>m<sup>2</sup>"
set-plot-option 3 S M 1 10<sup>-14</sup>m<sup>2</sup>
$ Renaming series in plot #4: #1 --> "10<sup>-14</sup>m<sup>2</sup>"
set-plot-option 4 S M 1 10<sup>-14</sup>m<sup>2</sup>
$ Renaming series in plot #5: #1 --> "10<sup>-14</sup>m<sup>2</sup>"
set-plot-option 5 S M 1 10<sup>-14</sup>m<sup>2</sup>
```

```
$ [S]pecial options, [d]iffusion in prec. is calculated from matrix diffusion with [r]atio of 0.01
set-precipitation-parameter CEMENTITE_PO S D R 0,01
$ In S[t]ructure, [d]islocations, [e]quilibrium dislocation density in ferrite domain set to 1e14
set-precipitation-parameter ferrite T D E 1e14
```


start-precipitate-simulation

set-gui-window-property . L

```
$----- Dislocation density 1e16 -----$
$ Renaming series in plot #1: #2 --> "10<sup>-16</sup>m<sup>2</sup>"
set-plot-option 1 S M 2 10<sup>-16</sup>m<sup>2</sup>
$ Renaming series in plot #2: #4 --> "10<sup>-16</sup>m<sup>2</sup>"
set-plot-option 2 S M 4 10<sup>-16</sup>m<sup>2</sup>
$ Renaming series in plot #2: #5 --> "10<sup>-16</sup>m<sup>2</sup>"
set-plot-option 2 S M 5 nucl_10<sup>-16</sup>m<sup>2</sup>
$ Renaming series in plot #3: #2 --> "10<sup>-16</sup>m<sup>2</sup>"
set-plot-option 3 S M 2 10<sup>-16</sup>m<sup>2</sup>
$ Renaming series in plot #4: #2 --> "10<sup>-16</sup>m<sup>2</sup>"
set-plot-option 4 S M 2 10<sup>-16</sup>m<sup>2</sup>
set-plot-option 4 A Y 1 Y log          $ Logarithmic scale on y-axis
$ Renaming series in plot #5: #2 --> "10<sup>-16</sup>m<sup>2</sup>"
set-plot-option 5 S M 2 10<sup>-16</sup>m<sup>2</sup>
```

```
$ In S[t]ructure, [d]islocations, [e]quilibrium dislocation density in ferrite domain set to 1e16
set-precipitation-parameter ferrite T D E 1e16
start-precipitate-simulation
```

```
$$*****
          SAVING WORKSPACE
*****$$
```

save-workspace Tutorial_15

SCRIPT TUTORIAL 16

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for effect of microstructure and conditions (Part 2) according to Tutorial 16.
 The following contents will be covered:

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

Database: mc_sample_fe.tdb
 Author: P. Warczok
 Creation date: 10.11.2008
 This is a script for MatCalc version 5.44 (rel 0.008)
 Last update: 26.09.2011 (G. Stechauner, Update for 5.44)

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module core \$ Use "core" module (MatCalc uses "core" module by default anyway)

read-workspace Tutorial_15 \$ Load Workspace from Tutorial 15

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$ verify correct MatCalc version (is accessible as internal variable)
if (matcalc_version<5440008)
  send-dialog-string "MatCalc version must be 5.44.0008 or higher to run this script. Stopping."
  stop-run-script $ stop script
endif
  
```

```

$$*****
***** SIMULTANEOUS PRECIPITATION WITH M23C6 *****
*****
  
```

```

create-new-phase M23C6 P          $ Creates M23C6 precipitate
set-precipitation-parameter M23C6_P0 C 25    $ Initializes M23C6 precipitate with 25 classes
set-precipitation-parameter M23C6_P0 N C O    $ Ortho-composition for the M23C6 precipitate nuclei
$ [G]rain boundaries are nucleation sites for M23C6 precipitate
set-precipitation-parameter M23C6_P0 N S G
  
```

```

$ Equilibrium dislocation density for ferrite domain set to 1e12
set-precipitation-parameter ferrite T D E 1e12
  
```

```

set-gui-window-property 2 R          $ All locked series are [r]emoved from GUI-window no.3
set-gui-window-property . S S 1e-12  $ Default x-axis scale starts at 1e-12
clear-calc-buffer                    $ Calculation buffer is cleared
  
```

```

set-plot-option 1 S N B F$M23C6_P0 %s    $ Plotting fraction of M23C6 precipitate phase
set-plot-option 1 A Y 1 T Phase fraction  $ y-axis title
set-plot-option 2 S R 1                    $ [R]emoves series no.1 in plot #1
set-plot-option 2 S N B X$BCC_A2$CR %s    $ Plotting Cr content in bcc phase
  
```

set-plot-option 4 S N B NUM_PREC\$M23C6_P0 %s \$ Plotting the number of particles of M23C6 precipitate
 set-plot-option 5 S N B R_MEAN\$M23C6_P0 %s \$ Plotting mean radius of M23C6 precipitates

set-plot-option 1 S M 0 Cementite \$ Renaming series in plot #1: #0 --> "Cementite"
 \$ Renaming series in plot #1: #1 --> "M₂₃C₆"
 set-plot-option 1 S M 1 M₂₃C₆
 set-plot-option 2 S M 0 Cementite \$ Renaming series in plot #2: #0 --> "Cementite"
 set-plot-option 2 S M 1 'Matrix (bcc_a2)' \$ Renaming series in plot #2: #1 --> "Matrix (bcc_a2)"
 \$ Renaming series in plot #3: #0 --> "X_{BCC_A2,C}"
 set-plot-option 3 S M 0 X_{BCC_A2,C}
 set-plot-option 4 S M 0 Cementite \$ Renaming series in plot #4: #0 --> "Cementite"
 \$ Renaming series in plot #4: #1 --> "M₂₃C₆"
 set-plot-option 4 S M 1 M₂₃C₆
 set-plot-option 5 S M 0 Cementite \$ Renaming series in plot #5: #0 --> "Cementite"
 \$ Renaming series in plot #5: #1 --> "M₂₃C₆"
 set-plot-option 5 S M 1 M₂₃C₆

set-simulation-parameter E 3,6e10 \$ End time - 3.6e10 seconds
 set-simulation-parameter T I 600 \$ Isothermal treatment at 600
 set-simulation-parameter P Y \$ Temperature in Celsius
 start-precipitate-simulation

\$\$*****
 EFFECT OF DISLOCATION DENSITY
 *****\$\$

\$ Renaming series in plot #1: #0 --> "Cementite, 10¹²m⁻², 10⁻⁴ m"
 set-plot-option 1 S M 0 'Cementite, 10¹²m⁻², 10⁻⁴ m'
 \$ Renaming series in plot #1: #1 --> "M₂₃C₆, 10¹²m⁻², 10⁻⁴ m"
 set-plot-option 1 S M 1 'M₂₃C₆, 10¹²m⁻², 10⁻⁴ m'
 \$ Renaming series in plot #2: #0 --> "Cementite, 10¹²m⁻², 10⁻⁴ m"
 set-plot-option 2 S M 0 'Cementite, 10¹²m⁻², 10⁻⁴ m'
 \$ Renaming series in plot #2: #1 --> "Matrix (bcc_a2), 10¹²m⁻², 10⁻⁴ m"
 set-plot-option 2 S M 1 'Matrix (bcc_a2), 10¹²m⁻², 10⁻⁴ m'
 \$ Renaming series in plot #3: #0 --> "X_{BCC_A2,C}, 10¹²m⁻², 10⁻⁴ m"
 set-plot-option 3 S M 0 'X_{BCC_A2,C}, 10¹²m⁻², 10⁻⁴ m'
 \$ Renaming series in plot #4: #0 --> "Cementite, 10¹²m⁻², 10⁻⁴ m"
 set-plot-option 4 S M 0 'Cementite, 10¹²m⁻², 10⁻⁴ m'
 \$ Renaming series in plot #4: #1 --> "M₂₃C₆, 10¹²m⁻², 10⁻⁴ m"
 set-plot-option 4 S M 1 'M₂₃C₆, 10¹²m⁻², 10⁻⁴ m'
 \$ Renaming series in plot #5: #0 --> "Cementite, 10¹²m⁻², 10⁻⁴ m"
 set-plot-option 5 S M 0 'Cementite, 10¹²m⁻², 10⁻⁴ m'
 \$ Renaming series in plot #5: #1 --> "M₂₃C₆, 10¹²m⁻², 10⁻⁴ m"
 set-plot-option 5 S M 1 'M₂₃C₆, 10¹²m⁻², 10⁻⁴ m'

set-gui-window-property . L \$ Locking all unlocked series
 \$ Renaming series in plot #1: #2 --> "Cementite, 10¹⁴m⁻², 10⁻⁴ m"
 set-plot-option 1 S M 2 'Cementite, 10¹⁴m⁻², 10⁻⁴ m'
 \$ Renaming series in plot #1: #3 --> "M₂₃C₆, 10¹⁴m⁻², 10⁻⁴ m"
 set-plot-option 1 S M 3 'M₂₃C₆, 10¹⁴m⁻², 10⁻⁴ m'
 \$ Renaming series in plot #2: #2 --> "Cementite, 10¹⁴m⁻², 10⁻⁴ m"
 set-plot-option 2 S M 2 'Cementite, 10¹⁴m⁻², 10⁻⁴ m'
 \$ Renaming series in plot #2: #3 --> "Matrix (bcc_a2), 10¹⁴m⁻², 10⁻⁴ m"
 set-plot-option 2 S M 3 'Matrix (bcc_a2), 10¹⁴m⁻², 10⁻⁴ m'
 \$ Renaming series in plot #3: #1 --> "X_{BCC_A2,C}, 10¹⁴m⁻², 10⁻⁴ m"
 set-plot-option 3 S M 1 'X_{BCC_A2,C}, 10¹⁴m⁻², 10⁻⁴ m'
 \$ Renaming series in plot #4: #2 --> "Cementite, 10¹⁴m⁻², 10⁻⁴ m"
 set-plot-option 4 S M 2 'Cementite, 10¹⁴m⁻², 10⁻⁴ m'

```
$ Renaming series in plot #4: #3 --> "M<sub>23</sub>C<sub>6</sub>, 10<sup>14</sup>m<sup>-2</sup>, 10<sup>-4</sup>m"
set-plot-option 4 S M 3 'M<sub>23</sub>C<sub>6</sub>, 10<sup>14</sup>m<sup>-2</sup>, 10<sup>-4</sup>m'
$ Renaming series in plot #5: #2 --> "Cementite, 10<sup>14</sup>m<sup>-2</sup>, 10<sup>-4</sup>m"
set-plot-option 5 S M 2 'Cementite, 10<sup>14</sup>m<sup>-2</sup>, 10<sup>-4</sup>m'
$ Renaming series in plot #5: #3 --> "M<sub>23</sub>C<sub>6</sub>, 10<sup>14</sup>m<sup>-2</sup>, 10<sup>-4</sup>m"
set-plot-option 5 S M 3 'M<sub>23</sub>C<sub>6</sub>, 10<sup>14</sup>m<sup>-2</sup>, 10<sup>-4</sup>m'

$ Dislocation density in ferrite domain set to 1e14
set-precipitation-parameter ferrite T D E 1e14
start-precipitate-simulation
```

```
$$*****
```

EFFECT OF GRAIN DIAMETER

```
*****$$
```

```
$ Renaming series in plot #1: #2 --> "Cementite, 10<sup>14</sup>m<sup>-2</sup>, 10<sup>-4</sup>m"
set-plot-option 1 S M 2 'Cementite, 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m'
$ Renaming series in plot #1: #3 --> "M<sub>23</sub>C<sub>6</sub>, 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m"
set-plot-option 1 S M 3 'M<sub>23</sub>C<sub>6</sub>, 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m'
$ Renaming series in plot #2: #2 --> "Cementite, 10<sup>14</sup>m<sup>-2</sup>, 10<sup>-4</sup>m"
set-plot-option 2 S M 2 'Cementite, 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m'
$ Renaming series in plot #2: #3 --> "Matrix (bcc_a2), 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m"
set-plot-option 2 S M 3 'Matrix (bcc_a2), 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m'
$ Renaming series in plot #3: #1 --> "X<sub>BCC_A2,C</sub>, 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m"
set-plot-option 3 S M 1 'X<sub>BCC_A2,C</sub>, 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m'
$ Renaming series in plot #4: #2 --> "Cementite, 10<sup>14</sup>m<sup>-2</sup>, 10<sup>-4</sup>m"
set-plot-option 4 S M 2 'Cementite, 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m'
$ Renaming series in plot #4: #3 --> "M<sub>23</sub>C<sub>6</sub>, 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m"
set-plot-option 4 S M 3 'M<sub>23</sub>C<sub>6</sub>, 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m'
$ Renaming series in plot #5: #2 --> "Cementite, 10<sup>14</sup>m<sup>-2</sup>, 10<sup>-4</sup>m"
set-plot-option 5 S M 2 'Cementite, 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m'
$ Renaming series in plot #5: #3 --> "M<sub>23</sub>C<sub>6</sub>, 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m"
set-plot-option 5 S M 3 'M<sub>23</sub>C<sub>6</sub>, 10<sup>12</sup>m<sup>-2</sup>, 10<sup>-5</sup>m'

$ Dislocation density in ferrite domain set to 1e12
set-precipitation-parameter ferrite T D E 1e12
$ In S[t]ructure, [g]rain size section, the grain diameter is set to 10e-6
set-precipitation-parameter ferrite T G 10e-6
start-precipitate-simulation
```

```
$$*****
```

SUBGRAINS AND ELONGATION FACTORS

```
*****$$
```

```
$----- Subgrains -----$
set-gui-window-property . R $ All locked series are [r]emoved from the current GUI-window[.]
$ Renaming series in plot #1: #0 --> "Cementite, g.b.(10<sup>-5</sup>m)"
set-plot-option 1 S M 0 'Cementite, g.b.(10<sup>-5</sup>m)'
$ Renaming series in plot #1: #1 --> "M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)"
set-plot-option 1 S M 1 'M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)'
$ Renaming series in plot #2: #0 --> "Cementite, g.b.(10<sup>-5</sup>m)"
set-plot-option 2 S M 0 'Cementite, g.b.(10<sup>-5</sup>m)'
$ Renaming series in plot #2: #1 --> "Matrix (bcc_a2), g.b.(10<sup>-5</sup>m)"
set-plot-option 2 S M 1 'Matrix (bcc_a2), g.b.(10<sup>-5</sup>m)'
$ Renaming series in plot #3: #0 --> "X<sub>BCC_A2,C</sub>, g.b.(10<sup>-5</sup>m)"
set-plot-option 3 S M 0 'X<sub>BCC_A2,C</sub>, g.b.(10<sup>-5</sup>m)'
```

```

$ Renaming series in plot #4: #0 --> "Cementite, g.b.(10<sup>-5</sup>m)m"
set-plot-option 4 S M 0 'Cementite, g.b.(10<sup>-5</sup>m)'
$ Renaming series in plot #4: #1 --> "M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)"
set-plot-option 4 S M 1 'M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)'
$ Renaming series in plot #5: #0 --> "Cementite, g.b.(10<sup>-5</sup>m)m"
set-plot-option 5 S M 0 'Cementite, g.b.(10<sup>-5</sup>m)'
$ Renaming series in plot #5: #1 --> "M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)"
set-plot-option 5 S M 1 'M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)'

set-gui-window-property . L      $ Locking all unlocked series
$ Renaming series in plot #1: #2 --> "Cementite, g.b.(10<sup>-5</sup>m)+sg.b."
set-plot-option 1 S M 2 'Cementite, g.b.(10<sup>-5</sup>m)+sg.b.'
$ Renaming series in plot #1: #3 --> "M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)+sg.b."
set-plot-option 1 S M 3 'M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)+sg.b.'
$ Renaming series in plot #2: #2 --> "Cementite, g.b.(10<sup>-5</sup>m)+sg.b."
set-plot-option 2 S M 2 'Cementite, g.b.(10<sup>-5</sup>m)+sg.b.'
$ Renaming series in plot #2: #3 --> "Matrix (bcc_a2), g.b.(10<sup>-5</sup>m)+sg.b."
set-plot-option 2 S M 3 'Matrix (bcc_a2), g.b.(10<sup>-5</sup>m)+sg.b.'
$ Renaming series in plot #3: #1 --> "X<sub>BCC_A2,C</sub>, g.b.(10<sup>-5</sup>m)+sg.b."
set-plot-option 3 S M 1 'X<sub>BCC_A2,C</sub>, g.b.(10<sup>-5</sup>m)+sg.b.'
$ Renaming series in plot #4: #2 --> "Cementite, g.b.(10<sup>-5</sup>m)+sg.b."
set-plot-option 4 S M 2 'Cementite, g.b.(10<sup>-5</sup>m)+sg.b.'
$ Renaming series in plot #4: #3 --> "M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)+sg.b."
set-plot-option 4 S M 3 'M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)+sg.b.'
$ Renaming series in plot #5: #2 --> "Cementite, g.b.(10<sup>-5</sup>m)+sg.b."
set-plot-option 5 S M 2 'Cementite, g.b.(10<sup>-5</sup>m)+sg.b.'
$ Renaming series in plot #5: #3 --> "M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)+sg.b."
set-plot-option 5 S M 3 'M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)+sg.b.'

```

```

$ [G]rain and [s]ubgrain boundaries are nucleation sites for M23C6 precipitate
set-precipitation-parameter M23C6_P0 N S GS
start-precipitate-simulation

```

```

$----- Elongation factors -----$
set-gui-window-property . L
$ Renaming series in plot #1: #4 --> "Cementite, g.b.(10<sup>-5</sup>m)+elong.sg.b."
set-plot-option 1 S M 4 'Cementite, g.b.(10<sup>-5</sup>m)+elong.sg.b.'
$ Renaming series in plot #1: #5 --> "M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)+elong.sg.b."
set-plot-option 1 S M 5 'M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)+elong.sg.b.'
$ Renaming series in plot #2: #4 --> "Cementite, g.b.(10<sup>-5</sup>m)+elong.sg.b."
set-plot-option 2 S M 4 'Cementite, g.b.(10<sup>-5</sup>m)+elong.sg.b.'
$ Renaming series in plot #2: #5 --> "Matrix (bcc_a2), g.b.(10<sup>-5</sup>m)+elong.sg.b."
set-plot-option 2 S M 5 'Matrix (bcc_a2), g.b.(10<sup>-5</sup>m)+elong.sg.b.'
$ Renaming series in plot #3: #2 --> "X<sub>BCC_A2,C</sub>, g.b.(10<sup>-5</sup>m)+elong.sg.b."
set-plot-option 3 S M 2 'X<sub>BCC_A2,C</sub>, g.b.(10<sup>-5</sup>m)+elong.sg.b.'
$ Renaming series in plot #4: #4 --> "Cementite, g.b.(10<sup>-5</sup>m)+elong.sg.b."
set-plot-option 4 S M 4 'Cementite, g.b.(10<sup>-5</sup>m)+elong.sg.b.'
$ Renaming series in plot #4: #5 --> "M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)+elong.sg.b."
set-plot-option 4 S M 5 'M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)+elong.sg.b.'
set-plot-option 4 A Y 1 Y lin      $ Linear scale on y-axis
$ Renaming series in plot #5: #4 --> "Cementite, g.b.(10<sup>-5</sup>m)+elong.sg.b."
set-plot-option 5 S M 4 'Cementite, g.b.(10<sup>-5</sup>m)+elong.sg.b.'
$ Renaming series in plot #5: #5 --> "M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)+elong.sg.b."
set-plot-option 5 S M 5 'M<sub>23</sub>C<sub>6</sub>, g.b.(10<sup>-5</sup>m)+elong.sg.b.'

```

```

$ Grain size e[l]ongation factor for ferrite domain is set to 10
set-precipitation-parameter ferrite T L 10
start-precipitate-simulation

```

```

$$*****

```

SAVING WORKSPACE

*****\$\$

save-workspace Tutorial_16

SCRIPT TUTORIAL 17

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for complex multi-stage heat treatments according to Tutorial 17.
 The following contents will be covered:

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

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 1400C with linear cooling to room temperature. The austenitization treatment is carried out at 1100C 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.

Database: mc_sample_fe2.tdb
 Author: P. Warczok
 Creation date: 10.11.2008
 This is a script for MatCalc version 5.44 (rel 0.008)
 Last update: 26.09.2011 (G. Stechauner, Update for 5.44)

```

*****
***** SETUP INFORMATION *****
*****
  
```

use-module core \$ Use "core" module (MatCalc uses "core" module by default anyway)

new-workspace \$ creates a new workspace

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$ verify correct MatCalc version (is accessible as internal variable)
if (matcalc_version<5440008)
  send-dialog-string "MatCalc version must be 5.44.0008 or higher to run this script. Stopping."
  stop-run-script $ stop script
endif
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****
  
```

```

open-thermodyn-database mc_fe.tdb      $ Thermodynamic database: mc_sample_fe2.tdb
select-elements FE C NB VA             $ Components: Fe, C, Nb
select-phases BCC_A2 FCC_A1            $ Phases: bcc, fcc
read-thermodyn-database
  
```

```

set-reference-element FE
enter-composition WP C=0,1 NB=0,7      $ Composition: 0.1 wt.% C, 0.7 wt.% Nb
  
```

```

set-temperature-celsius 1000           $ Temperature 1000C
  
```

```

set-automatic-startvalues
calculate-equilibrium          $ Initial equilibrium

create-precipitation-domain austenite      $ Creates precipitation domain "austenite"
set-precipitation-parameter austenite X FCC_A1    $ Austenite domain structure: fcc
create-precipitation-domain ferrite        $ Creates precipitation domain "ferrite"
set-precipitation-parameter ferrite X BCC_A2      $ Ferrite domain structure: bcc

create-new-phase FCC_A1#01 P              $ Creates NbC precipitate

read-mobility-database mc_fe.ddb          $ Mobility (diffusion) database: mc_sample_fe.ddb

$----- Setup GUI -----$
new-gui-window p1
set-gui-window-property . S U Y          $ Use default x-axis
set-gui-window-property . S T Time [s]    $ Default x-axis title
set-gui-window-property . S Y log         $ Logarithmic scale on default x-axis
set-gui-window-property . S S 10..       $ Scaling limit for the default x-axis
set-gui-window-property . S L N          $ No legend for the plots with the default x-axis

set-plot-option . S N B T $C %s          $ Plotting the temperature in Celsius
set-plot-option . A Y 1 T Temperature [C] $ y-axis title

create-new-plot X .
set-plot-option . S N B F $FCC_A1#01_P0 %s $ Plotting the fraction of NbC precipitate phase
set-plot-option . A Y 1 T NbC phase fraction $ y-axis title

create-new-plot X .
set-plot-option . S N B R_MEAN $FCC_A1#01_P0 %s $ Plotting the mean radius of NbC precipitate phase
set-plot-option . A Y 1 T Mean radius [nm] $ y-axis title
set-plot-option . A Y 1 Y log             $ Logarithmic scale on y-axis
set-plot-option . A Y 1 S 0.1..          $ Scaling range for y-axis
set-plot-option . A Y 1 F 1e9            $ Multiplication factor for y-axis

create-new-plot X .
$ Plotting the number of particles for NbC precipitate phase
set-plot-option . S N B NUM_PREC $FCC_A1#01_P0 %s
set-plot-option . A Y 1 T Number density [m<sup>-3</sup>] $ y-axis title
set-plot-option . A Y 1 Y log             $ Logarithmic scale on y-axis
set-plot-option . A Y 1 S 1..            $ Scaling range for y-axis

set-plot-option 1 G M X Y                $ Switching on the major gridlines for x-axis for plot no. 1
set-plot-option 1 G M Y Y                $ Switching on the major gridlines for y-axis for plot no. 1
set-plot-option 2 G M X Y                $ Switching on the major gridlines for x-axis for plot no. 2
set-plot-option 2 G M Y Y                $ Switching on the major gridlines for y-axis for plot no. 2
set-plot-option 3 G M X Y                $ Switching on the major gridlines for x-axis for plot no. 3
set-plot-option 3 G M Y Y                $ Switching on the major gridlines for y-axis for plot no. 3
set-plot-option 4 G M X Y                $ Switching on the major gridlines for x-axis for plot no. 4
set-plot-option 4 G M Y Y                $ Switching on the major gridlines for y-axis for plot no. 4
set-gui-window-property . N 2            $ Arranging plots in 2 columns

$$*****
DEFINITION OF THE HEAT TREATMENT
*****$$

create-heat-treatment sample_ht          $ Creates the heat treatment sequence

append-ht-segment sample_ht              $ Adding a segment to the heat treatment sequence
$ In the current segment[.], [s]tart temperature is set 1400C
edit-ht-segment sample_ht . S 1400
$ In the current segment[.], the parameter set no.[1] is chosen with end temperature

```



```

600C and cooling rate 1K/s $$
edit-ht-segment sample_ht . 1 600 -1
$$ In the current segment[.], precipitation [d]omain is [n]ot inherited from the previous
segment. It is set to austenite $$
edit-ht-segment sample_ht . D N austenite

append-ht-segment sample_ht          $ Adding a segment to the heat treatment sequence
$$ In the current segment[.], the parameter pair no.[1] is chosen with end temperature 25C
and cooling rate 1K/s $$
edit-ht-segment sample_ht . 1 25 -1
$$ In the current segment[.], precipitation [d]omain is [n]ot inherited from the
previous segment. It is set to ferrite $$
edit-ht-segment sample_ht . D N ferrite

append-ht-segment sample_ht          $ New segment
edit-ht-segment sample_ht . 1 850 1   $ End temperature: 850C; Heating rate: 1K/s
$ In the current segment[.], for precipitation [d]omain the inheritance option is set to [y]es
edit-ht-segment sample_ht . D Y

append-ht-segment sample_ht          $ New segment
edit-ht-segment sample_ht . 1 1100 1   $ End temperature: 1100C; Heating rate: 1K/s
edit-ht-segment sample_ht . D N austenite $ Precipitation domain: Austenite

append-ht-segment sample_ht          $ New segment
$$ In the current segment[.], the parameter set no.[3] is chosen with end temperature
1100C and heating time 7200 seconds. $$
edit-ht-segment sample_ht . 3 1100 7200
$ In the current segment[.], for precipitation [d]omain the inheritance option is set to [y]es
edit-ht-segment sample_ht . D Y

append-ht-segment sample_ht          $ New segment
edit-ht-segment sample_ht . 1 600 -1   $ End temperature: 600C; Heating rate: -1K/s
edit-ht-segment sample_ht . D Y        $ Precipitation domain: inherited from previous

append-ht-segment sample_ht          $ New segment
edit-ht-segment sample_ht . 1 25 -1     $ End temperature: 25C; Heating rate: -1K/s
edit-ht-segment sample_ht . D N ferrite $ Precipitation domain: Ferrite

$$ In the segment no.[0], a line is added[+] to the p[r]e-seg script
(Grain boundaries as nucleation sites for NbC precipitate) $$
edit-ht-segment sample_ht 0 R +set-precipitation-parameter FCC_A1#01_P0 N S G
$$ In the segment no.[0], a line is added[+] to the p[o]st-seg script
(Grain boundaries and dislocations as nucleation sites for NbC precipitate) $$
edit-ht-segment sample_ht 0 O +set-precipitation-parameter FCC_A1#01_P0 N S DG

save-workspace Tutorial_17_init

$$*****
                PERFORM SIMULATION
*****$$

$ Temperature profile from defined [h]eat treatment "sample_ht" with the max. temperature step of 10
set-simulation-parameter T H sample_ht 10
start-precipitate-simulation

$$*****
                SIMULATION WITH SEPARATION OF PRECIPITATE POPULATIONS
*****$$

create-new-phase FCC_A1#01 P          $ Creates the second phase for NbC precipitate

```

```

$$ In the segment no.[0], a line is added[+] to the p[r]e-seg script
(none of the nucleation sites are selected for the second NbC precipitate) $$
edit-ht-segment sample_ht 0 R +set-precipitation-parameter FCC_A1#01_P1 N S N
$$ In the segment no.[0], a line is removed[-] from the p[o]st-seg script
(Grain boundaries and dislocations as nucleation sites for the first NbC precipitate) $$
edit-ht-segment sample_ht 0 O -set-precipitation-parameter FCC_A1#01_P0 N S DG
$$ In the segment no.[0], a line is added[+] to the p[o]st-seg script
(none of the nucleation sites are selected for the first NbC precipitate) $$
edit-ht-segment sample_ht 0 O +set-precipitation-parameter FCC_A1#01_P0 N S N
$$ Segment no.0, post-seg script, adding: Grain boundaries and dislocations as nucleation
sites for NbC precipitate $$
edit-ht-segment sample_ht 0 O +set-precipitation-parameter FCC_A1#01_P1 N S DG

start-precipitate-simulation

$ Plotting the fraction of the second NbC precipitate phase
set-plot-option 2 S N B F$FCC_A1#01_P1 %s
set-plot-option . A Y 1 Y log          $ Logarithmic scale on y-axis
set-plot-option . A Y 1 S 1e-10..      $ Scaling on y-axis starts from 1e-10
$ Plotting the mean radius of the second NbC precipitate phase
set-plot-option 3 S N B R_MEAN$FCC_A1#01_P1 %s
$ Plotting the number of particles for NbC precipitate phase
set-plot-option 4 S N B NUM_PREC$FCC_A1#01_P1 %s

$$$$*****
SIMULATION WITH PRECIPITATES WITH NUCLEATION RESTRICTED TO SELECTED DOMAIN
*****$$$$

$$ For the [n]ucleation of the FCC_A1#01_P0 precipitate, the option of the nucleation
restricted to [p]recipitate domain restricted is switched to [y]es. The domain is selected
to austenite $$

set-precipitation-parameter FCC_A1#01_P0 N P Y austenite

$$ For the [n]ucleation of the FCC_A1#01_P1 precipitate, the option of the nucleation
restricted to [p]recipitate domain restricted is switched to [y]es. The domain is selected
to ferrite $$

set-precipitation-parameter FCC_A1#01_P1 N P Y ferrite

set-precipitation-parameter FCC_A1#01_P0 N S G    $ Nucleation site for FCC_A1#01_P0: grain boundaries

$ In the segment no.[0], the content of the p[r]e-seg script is cleared [-]
edit-ht-segment sample_ht 0 R -

$ In the segment no.[0], the content of the p[o]st-seg script is cleared [-]
edit-ht-segment sample_ht 0 O -

SET_GUI_WINDOW_PROPERTY . L          $ Duplicate and lock all plot series

start-precipitate-simulation

$$$$*****
SAVING WORKSPACE
*****$$$$

save-workspace Tutorial_17

```

SCRIPT TUTORIAL 18

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script for plotting a TTP diagram according to Tutorial 18.
 The following contents will be covered:

- 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.

Database: mc_sample_fe.tdb
 Author: P. Warczok
 Creation date: 10.11.2008
 This is a script for MatCalc version 5.44 (rel 0.008)
 Last update: 26.09.2011 (G. Stechauner, Update for 5.44)

```

*****
***** SETUP INFORMATION *****
*****$$
  
```

use-module core \$ Use "core" module (MatCalc uses "core" module by default anyway)

new-workspace \$ creates a new workspace

```

$$*****
***** SYSTEM SETUP *****
*****$$
  
```

```

$ verify correct MatCalc version (is accessible as internal variable)
if (matcalc_version<5440008)
  send-dialog-string "MatCalc version must be 5.44.0008 or higher to run this script. Stopping."
  stop-run-script $ stop script
endif
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****$$
  
```

```

open-thermodyn-database mc_fe.tdb      $ Thermodynamic database: mc_sample_fe.tdb
select-elements FE C NB VA             $ Components: Fe, C, Nb
select-phases BCC_A2 FCC_A1            $ Phases: bcc, fcc
read-thermodyn-database

set-reference-element FE
enter-composition WP C=0,1 NB=0,7      $ Composition: 0.1 wt.% C, 0.7 wt.% Nb

set-temperature-celsius 1000           $ Temperature 1000C
set-automatic-startvalues
calculate-equilibrium
search-phase-boundary T BCC_A2         $ Varying temperature for the bcc phase boundary search
  
```

```
set-temperature-celsius 1200      $ Temperature 1000C
calculate-equilibrium
search-phase-boundary T BCC_A2    $ Varying temperature for the bcc phase boundary search
```

\$\$*****

SETTING UP PLOTS

*****\$\$

```
new-gui-window p1
set-gui-window-property . X T$C      $ Temperature in Celsius set as variable on x-axis
set-plot-option . A X 1 T Temperature [C]      $ x-axis title
set-plot-option . A Y 1 T Equilibrium phase fraction of NbC $ y-axis title
set-plot-option . L N                  $ No legend
set-plot-option . S N B F$FCC_A1#01 %s        $ Plotting the fraction of NbC phase
```

```
set-step-option Y T      $ "Temperature" type
set-step-option R 1420 920 L 10      $ Range 920 - 1420; linear step of 10
set-step-option O C Y      $ Temperature in Celsius
step-equilibrium
```

```
set-plot-option 1 S L * Y      $ Lock all Series in Plot 1
set-gui-window-property . X stepvalue
```

```
create-precipitation-domain austenite
set-precipitation-parameter austenite X FCC_A1
```

```
create-new-phase FCC_A1#01 P
set-precipitation-parameter FCC_A1#01_P0 C 25
set-precipitation-parameter FCC_A1#01_P0 N S D
```

```
read-mobility-database mc_fe.ddb
```

\$\$*****

PRECIPITATION CALCULATION

*****\$\$

```
set-simulation-parameter E 1e5
set-simulation-parameter T I 925
start-precipitate-simulation
```

```
create-new-plot X .
set-plot-option . A X 1 T Time [s]
set-plot-option . A X 1 Y log
set-plot-option . A X 1 S 1..
set-plot-option . A Y 1 T NbC phase fraction
set-plot-option . L R
set-plot-option . S N B F$FCC_A1#01_P0 %s
set-gui-window-property . L
set-plot-option . S M -1 * _F$FCC_A1#01_P0 925C
```

```
set-simulation-parameter U 2
set-simulation-parameter E 1e5
set-simulation-parameter T I 1025
start-precipitate-simulation
set-gui-window-property . L
set-plot-option . S M -1 * _F$FCC_A1#01_P0 1025C
```

```
set-simulation-parameter E 1e5
set-simulation-parameter T I 1125
start-precipitate-simulation
set-gui-window-property . L
```

```
set-plot-option . S M -1 *_F$FCC_A1#01_P0 1125C
```

```
set-simulation-parameter U 2
set-simulation-parameter E 1e5
set-simulation-parameter T I 1175
start-precipitate-simulation
set-gui-window-property . L
set-plot-option . S M -1 *_F$FCC_A1#01_P0 1175C
```

```
set-simulation-parameter U 5
set-simulation-parameter E 1e5
set-simulation-parameter T I 1225
start-precipitate-simulation
set-plot-option . S L -1 F$FCC_A1#01_P0 Y
set-plot-option . S M -1 *_F$FCC_A1#01_P0 1225C
```

```
$\$*****
PLOTING THE TTP DIAGRAMS
*****$$
```

```
set-ttp-parameter E 1e5
set-ttp-parameter T 1225
set-ttp-parameter O 925
set-ttp-parameter D 25
set-ttp-parameter N 0.1
start-ttp-simulation
```

```
new-gui-window p6
set-plot-option . P R R
set-plot-option . S N D FCC_A1#01_P0 0.05
set-plot-option . S N D FCC_A1#01_P0 0.5
set-plot-option . S N D FCC_A1#01_P0 0.95
set-plot-option . S M 0 0.05
set-plot-option . S M 1 0.5
set-plot-option . S M 2 0.95
set-plot-option . A X 1 T Time [s]
set-plot-option . A Y 1 T Temperature [C]
```

```
set-plot-option . P R A
set-plot-option . S R *
set-plot-option . S N D FCC_A1#01_P0 1e-3
set-plot-option . S N D FCC_A1#01_P0 2e-3
set-plot-option . S N D FCC_A1#01_P0 3e-3
set-plot-option . S N D FCC_A1#01_P0 4e-3
set-plot-option . S N D FCC_A1#01_P0 5e-3
set-plot-option . S N D FCC_A1#01_P0 6e-3
set-plot-option . S N D FCC_A1#01_P0 7e-3
set-plot-option . S M 0 1e-3
set-plot-option . S M 1 2e-3
set-plot-option . S M 2 3e-3
set-plot-option . S M 3 4e-3
set-plot-option . S M 4 5e-3
set-plot-option . S M 5 6e-3
set-plot-option . S M 6 7e-3
```

```
set-plot-option . P R M
set-plot-option . S R *
set-plot-option . S N D FCC_A1#01_P0 0,1
set-plot-option . S N D FCC_A1#01_P0 0,2
set-plot-option . S N D FCC_A1#01_P0 0,3
set-plot-option . S N D FCC_A1#01_P0 0,4
set-plot-option . S N D FCC_A1#01_P0 0,5
```

```
set-plot-option . S N D FCC_A1#01_P0 0,6
set-plot-option . S N D FCC_A1#01_P0 0,7
set-plot-option . S N D FCC_A1#01_P0 0,8
set-plot-option . S N D FCC_A1#01_P0 0,9
set-plot-option . S M 0 0.1
set-plot-option . S M 1 0.2
set-plot-option . S M 2 0.3
set-plot-option . S M 3 0.4
set-plot-option . S M 4 0.5
set-plot-option . S M 5 0.6
set-plot-option . S M 6 0.7
set-plot-option . S M 7 0.8
set-plot-option . S M 8 0.9
```

```
$$*****
      SAVING WORKSPACE
*****$$
```

```
save-workspace Tutorial_18
```

SCRIPT TUTORIAL 19

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Scripting precipitation calculations according to Tutorial 19.
 The following contents will be covered:

- Setting up precipitation domains
- Setting up precipitate phases
- Scripting a complex heat-treatment
- Modifying precipitation parameters during heat-treatment
- Plotting using scripts

The example used here uses the already familiar Fe-Nb-C system and considers a heat-treatment of an initially well-annealed ferritic microstructure with no primary precipitates. Cementite is initially allowed to nucleate on dislocations, and NbC on grain boundaries. The microstructure is heated into the austenite phase stability region, held isothermally and then cooled quickly (quenched). On quenching, a martensitic transformation occurs. This is modelled in MatCalc by a modification of the ferrite precipitation domain to increase the dislocation density as well as the addition of subgrains as possible nucleation sites for the NbC phase. The system is then subjected to a tempering heat treatment consisting of heating, isothermal hold and cooling stages.

Database: mc_fe.tdb
 Author: V. Yardley
 Creation date: 20.02.2017
 This is a script for MatCalc version 6.00 (rel 0.100)
 Last update: M. Lueckl, 20.02.2017 - minor adjustments

```

*****
***** SETUP INFORMATION *****
*****$$
  
```

```

use-module core
close-workspace f          $ Close any open workspace without asking for save

new-workspace              $ creates a new workspace

if (matcalc_version<6000000)
  send-dialog-string "MatCalc version must be 6.00.0000 or higher to run this script. Stopping."
  stop-run-script
endif
  
```

```

@$*****
$ enter workspace info
@$*****
  
```

```

@ set-workspace-info Script T19
@ set-workspace-info +Calculation of precipitation
@ set-workspace-info +in Fe-0.1C-0,7Nb wt.% system
@ set-workspace-info +during a complex heat treatment
@ set-workspace-info +with phases BCC_A2, FCC_A1 and CEMENTITE.
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****$$
  
```

```

open-thermodyn-database mc_fe.tdb          $ Open thermodynamic database mc_fe.tdb
select-elements FE C NB VA                 $ Components: Fe, C, Nb, Va
  
```

Appendix A

select-phases BCC_A2 FCC_A1 CEMENTITE \$ Phases: bcc, fcc, cementite
read-thermodyn-database

set-reference-element Fe
enter-composition wp c=0.1 nb=0.7

read-mobility-database mc_fe.ddb \$ Mobility database

set-temperature-celsius 1000 \$ Temperature 1000C
set-automatic-startvalues
calculate-equilibrium \$ Initial equilibrium

\$\$*****

PRECIPITATION DOMAIN AND PHASES

*****\$\$

\$ ----- PRECIPITATION DOMAINS -----

create-precipitation-domain austenite \$ Create precipitation domain "austenite"
set-precipitation-parameter austenite X FCC_A1 \$ Austenite domain structure: fcc
\$ In S[t]ructure, [e]quilibrium)[d]islocation density set to 1e12
set-precipitation-parameter austenite T D E 1e12
\$ In S[t]ructure, [g]rain size section, the grain diameter is set to 100e-6
set-precipitation-parameter austenite T G 100e-6

create-precipitation-domain ferrite \$ Create precipitation domain "ferrite"
set-precipitation-parameter ferrite X BCC_A2 \$ Ferrite domain structure: bcc
\$ In S[t]ructure, [e]quilibrium)[d]islocation density set to 1e12
set-precipitation-parameter ferrite T D E 1e12
\$ In S[t]ructure, [g]rain diameter set to 100e-6
set-precipitation-parameter ferrite T G 100e-6
\$ In S[t]ructure, [s]ubgrain diameter is set to 10e-6
set-precipitation-parameter ferrite T S 10e-6
\$ In S[t]ructure, subgrain el[o]ngation factor set to 10
set-precipitation-parameter ferrite T O 10

\$ ----- PRECIPITATES -----

create-new-phase CEMENTITE P \$ Create precipitate
set-precipitation-parameter CEMENTITE_P0 C 100 \$ Size classes
\$ In the [n]ucleation section, the nucleation [s]ites are set to [d]islocations
set-precipitation-parameter CEMENTITE_P0 N S D
\$ In the [n]ucleation section, the nucleus [c]omposition is set to [p]ara-composition
set-precipitation-parameter CEMENTITE_P0 N C P

create-new-phase FCC_A1#01 P \$ Create precipitate
set-precipitation-parameter FCC_A1#01_P0 C 100 \$ Size classes
\$ [G]rain boundaries are [n]ucleation [s]ites for NbC precipitate
set-precipitation-parameter FCC_A1#01_P0 N S G
\$ [O]rtho-[c]omposition for the NbC precipitate [n]uclei
set-precipitation-parameter FCC_A1#01_P0 N C O

\$\$*****

THERMOMECHANICAL TREATMENT

*****\$\$

\$ ----- VARIABLES -----

set-variable-value f_a_temp 850 \$ ferrite-> austenite transformation temp. in C
set-variable-value a_f_temp 600 \$ austenite-> ferrite transformation temp. in C
set-variable-value aus_temp 1100 \$ austenitisation temp. in C

Appendix A

```

set-variable-value temp_temp 600          $ tempering temp. in C
set-variable-value rate_heat_to_aus 1     $ rate of heating to aus_temp in K/s
set-variable-value rate_cool_from_aus -10  $ rate of cooling from aus_temp in K/s
set-variable-value rate_heat_to_temp 1     $ rate of heating to temp_temp in K/s
set-variable-value rate_cool_from_temp -1  $ rate of cooling from temp_temp in K/s
set-variable-value aus_time 3600          $ austenitisation time in seconds
set-variable-value temp_time 7200        $ tempering time in seconds

$ ----- THERMOMECHANICAL TREATMENT -----

create-heat-treatment sample_ht

$ ----- AUSTENITISATION AND QUENCHING -----

append-ht-segment sample_ht              $ Adding a segment to the heat treatment sequence
edit-ht-segment sample_ht . S 20          $ Start temperature
edit-ht-segment sample_ht . 1 f_a_temp rate_heat_to_aus $ End temperature and heating rate
edit-ht-segment sample_ht . D N ferrite    $ Precipitation domain

append-ht-segment sample_ht              $ Adding a segment to the heat treatment sequence
edit-ht-segment sample_ht . 1 aus_temp rate_heat_to_aus $ End temperature and heating rate
edit-ht-segment sample_ht . D N austenite  $ Precipitation domain

append-ht-segment sample_ht              $ Adding a segment to the heat treatment sequence
edit-ht-segment sample_ht . 3 aus_temp aus_time $ End temperature and holding time
edit-ht-segment sample_ht . D Y           $ Precipitation domain is inherited

append-ht-segment sample_ht              $ Adding a segment to the heat treatment sequence
edit-ht-segment sample_ht . 1 a_f_temp rate_cool_from_aus $ End temperature and cooling rate
edit-ht-segment sample_ht . D Y           $ Precipitation domain is inherited

append-ht-segment sample_ht              $ Adding a segment to the heat treatment sequence
edit-ht-segment sample_ht . 1 20 rate_cool_from_aus $ End temperature and cooling rate
edit-ht-segment sample_ht . D N ferrite    $ Precipitation domain
edit-ht-segment sample_ht . O +set-precipitation-parameter ferrite T D E 1e14 $ Post-segment: Change the equilibrium
dislocation density
edit-ht-segment sample_ht . O +set-precipitation-parameter FCC_A1#01_P0 N S GS $ Post-segment: Change the nucleation
site

$ ----- TEMPERING -----

append-ht-segment sample_ht              $ Adding a segment to the heat treatment sequence
edit-ht-segment sample_ht . 1 temp_temp rate_heat_to_temp $ End temperature and heating rate
edit-ht-segment sample_ht . D Y           $ Precipitation domain is inherited

append-ht-segment sample_ht              $ Adding a segment to the heat treatment sequence
edit-ht-segment sample_ht . 3 temp_temp temp_time $ End temperature and holding time
edit-ht-segment sample_ht . D Y           $ Precipitation domain is inherited

append-ht-segment sample_ht              $ Adding a segment to the heat treatment sequence
edit-ht-segment sample_ht . 1 20 rate_cool_from_temp $ End temperature and cooling rate
edit-ht-segment sample_ht . D Y           $ Precipitation domain is inherited

$$*****
GRAPHICAL OUTPUT
*****$$

new-gui-window p1
set-gui-window-property . S U Y          $ Use default x-axis
set-gui-window-property . S T Time [h]   $ Default x-axis title
set-gui-window-property . S Y lin        $ Linear scale
set-gui-window-property . S S 1e-10..    $ Scaling limit x-axis

```

Appendix A

```

set-gui-window-property . S F 1/3600          $ Multiplication factor s -> h
set-plot-option . S N B T$C %s                $ Temperature in Celsius
set-plot-option . A Y 1 T Temperature [°C]     $ y-axis title
set-plot-option . L N                          $ No legend

create-new-plot X .
set-plot-option . A Y 1 T Phase fraction        $ y-axis title
$ New series: fraction of cementite precipitate phase
set-plot-option . S N B F$CEMENTITE_PO %s
$ New series: fraction of NbC precipitate phase
set-plot-option . S N B F$FCC_A1#01_PO %s
set-plot-option . S M 0 Cementite               $ Rename series -> "Cementite"
set-plot-option . S M 1 NbC                     $ Rename series -> "NbC"

create-new-plot X .
set-plot-option . A Y 1 T N<sub>ppt</sub> [m<sup>-3</sup>] $ y-axis title
set-plot-option . A Y 1 Y log                   $ Log scale on y-axis
set-plot-option . S N B NUM_PREC$CEMENTITE_PO %s
set-plot-option . S N B NUM_PREC$FCC_A1#01_PO %s
set-plot-option . S M 0 Cementite               $ Rename series in plot -> "Cementite"
set-plot-option . S M 1 NbC                     $ Rename series in plot -> "NbC"

create-new-plot X .
$ Plotting the mean radius
set-plot-option . A Y 1 T R<sub>mean</sub> [m]      $ y-axis title
set-plot-option . A Y 1 Y log                   $ Logarithmic scale on y-axis
set-plot-option 4 S N B R_MEAN$CEMENTITE_PO %s
set-plot-option 4 S N B R_MEAN$FCC_A1#01_PO %s
set-plot-option 4 S M 0 Cementite               $ Rename series in plot -> "Cementite"
set-plot-option 4 S M 1 NbC                     $ Rename series in plot --> "NbC"

$ Major gridlines for both x- and y-axes of all plots
set-plot-option 1 G M X Y
set-plot-option 1 G M Y Y
set-plot-option 2 G M X Y
set-plot-option 2 G M Y Y
set-plot-option 3 G M X Y
set-plot-option 3 G M Y Y
set-plot-option 4 G M X Y
set-plot-option 4 G M Y Y

new-gui-window p5                                $ Histogram
set-gui-window-property . S U Y                  $ Use default x-axis
set-gui-window-property . S T Precipitate radius [nm] $ x-axis title
set-gui-window-property . S F 1e9                $ Multiplication [f]actor
set-plot-option . S N P CEMENTITE_PO             $ New series
set-plot-option . H N 20                         $ [n]umber of [h]istogram classes set to 20
set-plot-option . T Cementite precipitate distribution $ plot title
set-plot-option . A Y 1 T Number density of precipitates [m<sup>-3</sup>] $ y-axis title
set-plot-option . L N                            $ [N]o legend box

new-gui-window p5                                $ Histogram
set-gui-window-property . S U Y                  $ Use default x-axis
set-gui-window-property . S T Precipitate radius [nm] $ x-axis title
set-gui-window-property . S F 1e9                $ Multiplication [f]actor
set-plot-option . S N P FCC_A1#01_PO             $ New series
set-plot-option . H N 20                         $ number of classes
set-plot-option . T NbC precipitate distribution $ plot title
set-plot-option . A Y 1 T Number density of precipitates [m<sup>-3</sup>] $ y-axis title
set-plot-option . L N                            $ [N]o legend box

```

\$\$*****

KINETIC CALCULATION

*****\$\$

set-simulation-parameter E 7200 \$ Simulation end tim[e] in s
 set-simulation-parameter T I 600 \$ Isothermal - temperature
 set-simulation-parameter P Y \$ Tem[p]erature in Celsius
 start-precipitate-simulation

set-simulation-parameter T H sample_ht 10
 start-precipitate-simulation

\$\$*****

SAVING WORKSPACE

*****\$\$

save-workspace Tutorial_19

SCRIPT TUTORIAL 20

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script Simulating grain growth according to Tutorial 20.
 The following contents will be covered:

- using the single-class model for grain growth

Database: mc_fe.tdb
 Author: M. Lueckl
 Creation date: 16.02.2017
 This is a script for MatCalc version 6.00 (rel 0.100)
 Last update:

```

*****
***** SETUP INFORMATION *****
*****
  
```

```

use-module core          $ Select core module for kinetic simulation
close-workspace f        $ Close any open workspace without asking for save
  
```

```

new-workspace            $ Create a new workspace
  
```

```

$ Add some information about your Script
@ echo n
set-workspace-info Script T20
set-workspace-info +Simulating grain growth
set-workspace-info +using the single-class model
  
```

```

echo y
  
```

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$ verify correct MatCalc version (is accessible as internal variable)
if (matcalc_version<6000000)
  send-dialog-string "Sorry, MatCalc version must be 6.00.0000 or higher to run this script. The script stops now."
  stop_run_script $ stop script
endif
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****
  
```

```

open-thermodyn-database mc_fe.tdb          $ Open thermodynamic database mc_fe.tdb
  
```

```

select-elements FE          $ Components: Fe
select-phases BCC_A2        $ Phases: bcc
read-thermodyn-database
  
```

```

read-mobility-database mc_fe.ddb          $ Mobility (diffusion) database: mc_fe.ddb
  
```

```

set-temperature-celsius 1000          $ Temperature 1000C
set-automatic-startvalues
calculate-equilibrium                $ Initial equilibrium
  
```

```

$-----PRECIPITATION DOMAIN -----$
  
```

```

create-precipitation-domain ferrite      $ Creates precipitation domain "ferrite"
set-precipitation-parameter ferrite X BCC_A2    $ Ferrite domain structure: bcc
set-precipitation-parameter ferrite t g 100e-6  $ Domain grain size [m] (initial)
set-precipitation-parameter ferrite e g m s      $ In microstructure [e]volution, [g]rain structure [m]odel is set to [s]ingle
class
set-precipitation-parameter ferrite e g s d 2    $ In microstructure [e]volution, [g]rain structure [s]ingle class model, k_[d]-
parameter equals 2
set-precipitation-parameter ferrite e g s r 1.5  $ In microstructure [e]volution, [g]rain structure [s]ingle class model, k_[r]-
parameter equals 1,5

```

\$\$*****

SETTING UP PLOTS

*****\$\$

```

new-gui-window p1
set-gui-window-property . s u y      $ Use default x-axis for all plots: yes
set-gui-window-property . s t Time [h]  $ Default x-axis title
set-gui-window-property . s f 1/3600    $ X-axis scaling factor
set-plot-option . a y t Grain diameter [μm]  $ Y-axis title
set-plot-option . a y 1 s 100..        $ Y-axis scaling range
set-plot-option . a y 1 f 1e6          $ Y-axis scaling factor
set-plot-option . s n b GD$ferrite      $ Add series: mean grain diameter in domain
set-plot-option . l b                  $ Show legend at the bottom of the figure
move-gui-window . 0 200 400 600

```

\$\$*****

KINETIC CALCULATION

*****\$\$

```

$ Isothermal holding at 800°C
set-simulation-parameter e 36000      $ Set simulation [e]nd time
set-simulation-parameter p y          $ Temperature in celsius
set-simulation-parameter t i 800      $ Isothermal temperature
start-precipitate-simulation
set-gui-window-property . l          $ Duplicate an lock all series
set-plot-option . s m -1 *_gd$ferrite 800°C  $ Rename series

```

```

$ Isothermal holding at 750°C
set-simulation-parameter t i 750      $ Isothermal temperature
start-precipitate-simulation
set-gui-window-property . l          $ Duplicate an lock all series
set-plot-option . s m -1 *_gd$ferrite 750°C  $ Rename series

```

```

$ Isothermal holding at 700°C
set-simulation-parameter t i 700      $ Isothermal temperature
start-precipitate-simulation
set-plot-option . s m -1 gd$ferrite 700°C  $ Rename series

```

SCRIPT TUTORIAL 21

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script Strain induced precipitates according to Tutorial 21.
 The following contents will be covered:

- Introduction of deformation into the thermo-mechanical treatment
- Effect of volumetric misfit on precipitation kinetics
- Effects of the applied deformation on the precipitation kinetics

Deformation process influences the microstructure of the alloy. One of the effects is the occurrence of the strain induced precipitates. This tutorial demonstrates how the deformation processes can be included in the simulation of the processed material. Moreover, the effects of the deformation on the precipitation kinetics are demonstrated and discussed.

Database: mc_fe.tdb
 Author: M. Lueckl
 Creation date: 17.02.2017
 This is a script for MatCalc version 6.00 (rel 0.100)
 Last update:

```

*****
***** SETUP INFORMATION *****
*****$$
  
```

```

use-module core          $ Select core module for kinetic simulation
close-workspace f        $ Close any open workspace without asking for save
  
```

```

new-workspace            $ Create a new workspace
  
```

```

$ Add some information about your Script
@ echo n
set-workspace-info Script T20
set-workspace-info +Simulating grain growth
set-workspace-info +using the single-class model
  
```

```

echo y
  
```

```

$$*****
***** SYSTEM SETUP *****
*****$$
  
```

```

$ verify correct MatCalc version (is accessible as internal variable)
if (matcalc_version<5440008)
  send-dialog-string "MatCalc version must be 5.44.0008 or higher to run this script. Stopping."
  stop_run_script $ stop script
endif
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****$$
  
```

```

if (matcalc_version<6000000)
  open-thermodyn-database mc_sample_fe2.tdb    $ Open thermodynamic database mc_sample_fe2.tdb
else
  test-exist-td-database mc_fe.tdb
  if(test_result==1)
    open-thermodyn-database mc_fe.tdb          $ Open thermodynamic database mc_fe.tdb
  
```

Appendix A

```

else
    send-dialog-string ""mc_fe.tdb"-database not found. Please, download it from MatCalc Website"
endif
endif

select-elements Fe C Nb          $ Components: Fe, C, Nb
select-phases bcc_a2 fcc_a1 cementite    $ Phases: bcc, fcc, cementite
read-thermodyn-database

set-reference-element Fe
enter-composition wp c=0.2 nb=0.04

if (matcalc_version<6000000)
    read-mobility-database mc_sample_fe.ddb    $ Mobility (diffusion) database: mc_sample_fe.ddb
else
    test-exist-mob-database mc_fe.ddb
    if(test_result==1)
        read-mobility-database mc_fe.ddb    $ Opens thermodynamic database mc_fe.ddb
    else
        send-dialog-string ""mc_fe.ddb"-database not found. Please, download it from MatCalc Website"
    endif
endif

set-temperature-celsius 1000          $ Temperature 1000C
set-automatic-startvalues
calculate-equilibrium                $ Initial equilibrium

$$*****
                        STEPPED EQUILIBRIUM CALCULATIONS
*****$$

set-step-option Y T          $ Select the t[y]pe of calculation: "[T]emperature"
set-step-option R 1400 400 L 10    $ Define the temperature range and the step
set-step-option O C Y          $ Temperature in celsius
step-equilibrium              $ Performs stepped equilibrium calculation

$$*****
                        GRAPHICAL OUTPUT
*****$$

new-gui-window p1            $ Create plot window
move-gui-window . 150 100 600 500    $ Move and resize plot window

$ define default x-axis properties
set-gui-window-property . s u y          $ Use default x-axis for all plots
set-gui-window-property . s t temperature / °C    $ Axis title
set-gui-window-property . x T$C          $ X-axis data

$ define plot properties: phase fraction
set-plot-option . a y 1 t phase fraction    $ Axis title
set-plot-option . s n b f$*          $ Add series
set-plot-option . a y 1 y log          $ Type: log

update-gui-window .          $ Update the GUI window
set-gui-window-property . l          $ Duplicate and lock all series

$ Remove all duplicated series
set-plot-option 1 s r -1 f$fcc_a1
set-plot-option 1 s r -1 f$fcc_a1#01
set-plot-option 1 s r -1 f$bcc_a2
set-plot-option 1 s r -1 f$cementite

```

```

$$*****
PRECIPITATION DOMAIN AND PHASES
*****$$

$ ----- PRECIPITATION DOMAIN -----
create-precipitation-domain austenite          $ Creates precipitation domain "austenite"
set-precipitation-parameter austenite x fcc_a1  $ Austenite domain structure: fcc

$ ----- PRECIPITATE -----
create-new-phase fcc_a1#01 p                   $ Creates NbC precipitate
set-precipitation-parameter fcc_a1#01_p0 n s d  $ Nucleation sites at dislocations

$$*****
THERMOMECHANICAL TREATMENT
*****$$

create-heat-treatment cooling                   $ Create the heat treatment sequence

append-ht-segment cooling                      $ Adding a segment to the heat treatment sequence
edit-ht-segment cooling . S 1300                $ Start temperature is set 1300C
edit-ht-segment cooling . 1 750 -1             $ End temperature and cooling rate
edit-ht-segment cooling . D N austenite         $ Precipitation domain

$$*****
GRAPHICAL OUTPUT
*****$$

new-gui-window p1                             $ Create plot window
move-gui-window . 75 15 880 790               $ Move and resize plot window

$ Define default x-axis properties
set-gui-window-property . s u y                $ Use default x-axis for all plots
set-gui-window-property . s t time / s         $ Axis title
set-gui-window-property . s y lin              $ Type: lin
set-gui-window-property . s s 1                $ X-axis scaling
set-gui-window-property . n 2                  $ Two plot columns

$ Define plot properties: temperature profile
set-plot-option . a y 1 t temperature / C      $ Axis title
set-plot-option . s n b T$c                    $ Add series
set-plot-option . g m y y                      $ Y-Axis major gridlines
set-plot-option . g m x y                      $ X-Axis major gridlines

$ Define plot properties: phase fraction
create-new-plot x .                            $ Create a new plot
set_plot_option . l a y                        $ Use kinetic alias name
set-plot-option . a y 1 t phase fraction        $ Axis title
set-plot-option . a y 1 y log                  $ Log scale
set-plot-option . a y 1 s 1e-10..0.001         $ Rescale axis
set-plot-option . s n b f_prec$*              $ Add series
set-plot-option . g m y y                      $ Y-Axis major gridlines
set-plot-option . g m x y                      $ X-Axis major gridlines

$ Define plot properties: number density
create-new-plot x .                            $ Create a new plot
set_plot_option . l a y                        $ Use kinetic alias name
set-plot-option . a y 1 t number density / m<sup>-3</sup> $ Axis title
set-plot-option . a y 1 y log                  $ Log scale
set-plot-option . a y 1 s 1e16..2e21           $ Rescale axis

```



```
set-plot-option . s n b num_prec$*      $ Add series
set-plot-option . g m y y                $ Y-Axis major gridlines
set-plot-option . g m x y                $ X-Axis major gridlines
```

```
$ Define plot properties: mean radius
create-new-plot x .                      $ Create a new plot
set_plot_option . l a y                  $ Use kinetic alias name
set-plot-option . a y 1 t mean radius / nm $ Axis title
set-plot-option . a y 1 y log            $ Log scale
set-plot-option . a y 1 s 0.6..10        $ Rescale axis
set-plot-option . a y 1 f 1e9             $ Factor -> nm
set-plot-option . s n b r_mean$*         $ Add series
set-plot-option . g m y y                $ Y-Axis major gridlines
set-plot-option . g m x y                $ X-Axis major gridlines
```

```
$$*****
      KINETIC CALCULATION
*****$$
```

```
set-simulation-parameter t h cooling 10    $ Define the max. temperature step
start-precipitate-simulation
```

```
set-gui-window-property 3 l              $ Duplicate an lock all series
```

```
set-plot-option 2 s m -1 *_T$C Cooling    $ Rename series
set-plot-option 3 s m -1 fcc_a1#01_p0 NbC $ Rename series
set-plot-option 4 s m -1 fcc_a1#01_p0 NbC $ Rename series
set-plot-option 5 s m -1 fcc_a1#01_p0 NbC $ Rename series
```

```
rename-current-buffer cooling             $ Give the buffer a new name
```

```
$$*****
      EFFECT OF VOLUMETRIC MISFIT
*****$$
```

```
create-calc-buffer Vol_misfit             $ Create a new buffer
set-gui-window-property 3 b Vol_misfit    $ Assign the buffer to the plot
```

```
$ ----- PRECIPITATE -----
set-precipitation-parameter fcc_a1#01_p0 t m n 0,1 $ Use volumetric misfit between prec./matrix
set-precipitation-parameter fcc_a1#01_p0 N F Y      $ Take volumetric misfit into account during nucleation
```

```
$ ----- KINETIC CALCULATION -----
set-simulation-parameter t h cooling 10    $ Define the max. temperature step
start-precipitate-simulation
set-gui-window-property 3 l              $ Duplicate an lock all series
```

```
set-plot-option 2 s m -1 *_T$C Cooling    $ Rename series
set-plot-option 3 s m -1 fcc_a1#01_p0 NbC(misfit) $ Rename series
set-plot-option 4 s m -1 fcc_a1#01_p0 NbC(misfit) $ Rename series
set-plot-option 5 s m -1 fcc_a1#01_p0 NbC(misfit) $ Rename series
```

```
$$*****
      SIMULATION OF DEFORMATION PROCESS
*****$$
```

```
create-calc-buffer Deformation             $ Create a new buffer
set-gui-window-property 3 b Deformation    $ Assign the buffer to the plot
```

```
$ ----- PRECIPITATION DOMAIN -----
```

```

set-precipitation-parameter austenite e s m s      $ Sherstnev-Kozeschnik simple

$ ----- PRECIPITATE -----
set-precipitation-parameter fcc_a1#01_p0 N I Y    $ Ignore volumetric misfit during deformation

$ ----- THERMOMECHANICAL TREATMENT -----
create-heat-treatment deformation                $ Create the heat treatment sequence

append-ht-segment deformation                    $ Adding a segment to the heat treatment sequence
edit-ht-segment deformation . S 1300             $ Start temperature is set 1300C
edit-ht-segment deformation . 1 1000 -1          $ End temperature and cooling rate
edit-ht-segment deformation . D N austenite      $ Precipitation domain

append-ht-segment deformation                    $ Adding a segment to the heat treatment sequence
$ In the current segment [.], the parameter pair no.[4] is chosen with accumulated strain of 0.7
edit-ht-segment deformation . 4 0.7             $ Accumulated strain
$ In the current segment [.], eps dot with 0.15 is chosen
edit-ht-segment deformation . e 0.15            $ eps dot
edit-ht-segment deformation . D N austenite      $ Precipitation domain

append-ht-segment deformation                    $ Adding a segment to the heat treatment sequence
edit-ht-segment deformation . 1 950 -1          $ End temperature and cooling rate
edit-ht-segment deformation . D N austenite      $ Precipitation domain

append-ht-segment deformation                    $ Adding a segment to the heat treatment sequence
$ In the current segment [.], the parameter pair no.[4] is chosen with accumulated strain of 0.7
edit-ht-segment deformation . 4 0.7             $ Accumulated strain
$ In the current segment [.], eps dot with 0.15 is chosen
edit-ht-segment deformation . e 0.15            $ eps dot
edit-ht-segment deformation . D N austenite      $ Precipitation domain

append-ht-segment deformation                    $ Adding a segment to the heat treatment sequence
edit-ht-segment deformation . 1 900 -1          $ End temperature and cooling rate
edit-ht-segment deformation . D N austenite      $ Precipitation domain

append-ht-segment deformation                    $ Adding a segment to the heat treatment sequence
$ In the current segment [.], the parameter pair no.[4] is chosen with accumulated strain of 0.7
edit-ht-segment deformation . 4 0.7             $ Accumulated strain
$ In the current segment [.], eps dot with 0.15 is chosen
edit-ht-segment deformation . e 0.15            $ eps dot
edit-ht-segment deformation . D N austenite      $ Precipitation domain

append-ht-segment deformation                    $ Adding a segment to the heat treatment sequence
edit-ht-segment deformation . 1 750 -1          $ End temperature and cooling rate
edit-ht-segment deformation . D N austenite      $ Precipitation domain

$ ----- KINETIC CALCULATION -----
set-simulation-parameter t h deformation 10      $ Define the max. temperature step
start-precipitate-simulation

set-plot-option 2 s m -1 T$C Deformation         $ Rename series
set-plot-option 3 s m -1 fcc_a1#01_p0 NbC(deform) $ Rename series
set-plot-option 4 s m -1 fcc_a1#01_p0 NbC(deform) $ Rename series
set-plot-option 5 s m -1 fcc_a1#01_p0 NbC(deform) $ Rename series

update-gui-windows 3                            $ update the GUI window

$$*****
SAVING WORKSPACE
*****$$

save-workspace Tutorial_21

```

SCRIPT TUTORIAL 22

new-workspace

open-thermodynamic-database mc_fe.tdb
 select-elements c
 select-phases fcc_a1
 read-thermodynamic-database

read-mobility-database mc_fe.ddb

enter-composition weight-percent c=0,2

set-automatic-startvalues
 set-temperature-celsius 1000
 calculate-equilibrium

create-precipitation-domain matrix
 set-precipitation-parameter matrix thermodynamic-matrix-phase=FCC_A1
 set-precipitation-parameter matrix subgrain-evolution-model=abc

create-tm-treatment tmt
 append-tmt-segment tmt
 edit-tmt-segment tmt . segment-start-temperature=1200
 edit-tmt-segment tmt . segment-accumulated-strain=,1
 edit-tmt-segment tmt . deformation-rate=1
 edit-tmt-segment tmt . precipitation-domain=matrix

append-tmt-segment tmt
 edit-tmt-segment tmt . T_dot+delta_t 0 1e4
 edit-tmt-segment tmt . precipitation-domain=matrix

set-simulation-parameter temperature-control temperature-control-type=from-tm-treatment
 set-simulation-parameter tm-treatment-name=tmt
 start-precipitate-simulation

new-gui-window p1 \$ create plot window
 move-gui-window displace . 75 15 800 800 \$ move and resize plot window

\$ define default x-axis properties
 set-gui-window-property window-id=. default-x-axis-for-all-plots=yes
 set-gui-window-property window-id=. default-x-axis-data=stepvalue
 set-gui-window-property window-id=. default-x-axis-title="Time [s]"
 set-gui-window-property window-id=. default-x-axis-type=log
 set-gui-window-property window-id=. default-x-axis-scaling=1e-5..
 set-gui-window-property window-id=. default-x-axis-legend=bottom

set-gui-window-property . number-of-plot-columns=auto

\$ define plot properties: dislocation density
 set-plot-option . use-alias-names-in-legend=yes
 set-plot-option . y-axis-title="Dislocation density [m^{-2}]"
 set-plot-option . series new buffer DD_TOT\$*
 \$set-plot-option . series new buffer DD_EQU_RS\$*
 set-plot-option . series new buffer DD_EX_RS\$*
 set-plot-option . y-axis-type=log
 set-plot-option . grid major enable-x-axis=yes

```
set-plot-option . grid major enable-y-axis=yes
```

```
$ define plot properties: subgrain diameter
create-new-plot xy-plot .
set-plot-option . use-alias-names-in-legend=yes
set-plot-option . y-axis-title="Mean subgrain diameter [<html>&mu;m]"
set-plot-option . series new buffer SGD$*
set-plot-option . y-axis-factor=1e6
set-plot-option . y-axis-type=log
set-plot-option . grid major enable-x-axis=yes
set-plot-option . grid major enable-y-axis=yes
```

```
$ define plot properties: grain diameter
create-new-plot xy-plot .
set-plot-option . use-alias-names-in-legend=yes
set-plot-option . y-axis-title="Grain diameter [<html>&mu;m]"
set-plot-option . series new buffer GD$*
set-plot-option . y-axis-factor=1e6
set-plot-option . y-axis-type=log
```

```
set-plot-option . grid major enable-x-axis=yes
set-plot-option . grid major enable-y-axis=yes
```

```
rename-current-buffer deformation_only
create-calc-buffer deformation&growth
set-gui-window-property . buffer-name=deformation&growth
```

```
set-precipitation-parameter matrix grain-evolution-model=single-class
start-precipitate-simulation
```

```
create-calc-buffer recrystallization
set-gui-window-property . buffer-name=recrystallization
```

```
set-plot-option . series new buffer GD_DEF$*
set-plot-option . series new buffer GD_RX$*
set-plot-option . y-axis-scaling=..2000
```

```
$ define plot properties: Nucleation rate of recrystallized grains
create-new-plot xy-plot .
set-plot-option . use-alias-names-in-legend=yes
set-plot-option . y-axis-title="Nucl. rate of rex. grains [ $m^{-3}s^{-1}$ ]"
set-plot-option . series new buffer RX_NUCL_RATE$*
set-plot-option . y-axis-type=log
```

```
set-plot-option . grid major enable-x-axis=yes
set-plot-option . grid major enable-y-axis=yes
```

```
$ define plot properties: Nucleation density of grains
create-new-plot xy-plot .
set-plot-option . use-alias-names-in-legend=yes
set-plot-option . y-axis-title="Number density of grains [ $m^{-3}$ ]"
set-plot-option . series new buffer NG$*
set-plot-option . series new buffer NG_DEF$*
set-plot-option . series new buffer NG_RX$*
set-plot-option . y-axis-type=log
```

```
set-plot-option . grid major enable-x-axis=yes
```

```
set-plot-option . grid major enable-y-axis=yes
```

```
$ define plot properties: Recrystallized fraction
```

```
create-new-plot xy-plot .
```

```
set-plot-option . use-alias-names-in-legend=yes
```

```
set-plot-option . y-axis-title="Recrystallized fraction"
```

```
set-plot-option . series new buffer X_RX$*
```

```
set-plot-option . grid major enable-x-axis=yes
```

```
set-plot-option . grid major enable-y-axis=yes
```

```
set-precipitation-parameter matrix allow-recrystallisation=yes
```

```
start-precipitate-simulation
```

SCRIPT TUTORIAL 23

```

$$*****
***** GENERAL INFORMATION *****
*****
  
```

Script cell simulations: long-range diffusion according to Tutorial 22.
 The following contents will be covered:

- setting up a simulation grid
- assigning properties to cells
- setting up display of cell simulation results
- setting up simulation parameters
- boundary conditions

Database: mc_fe.tdb
 Author: V. Yardley
 Creation date: 14.02.2017
 This is a script for MatCalc version 6.00 (rel 0.200)
 Last update: M. Lueckl, 14.02.2017 - minor adjustments

```

*****
***** SETUP INFORMATION *****
*****
  
```

```

use-module core          $ Select core module for kinetic simulation
close-workspace f        $ Close any open workspace without asking for save

new-workspace            $ Create a new workspace
  
```

```

$ Add some information about your Script
@ echo n
set-workspace-info Script T22
set-workspace-info +Simulation of long-range diffusion of C
set-workspace-info +out of thin film
set-workspace-info +with matrix phase FCC_A1

echo y
  
```

```

$$*****
***** SYSTEM SETUP *****
*****
  
```

```

$ verify correct MatCalc version (is accessible as internal variable)
if (matcalc_version<5440008)
  send-dialog-string "MatCalc version must be 5.44.0008 or higher to run this script. Stopping."
  stop_run_script $ stop script
endif
  
```

```

$$*****
***** DATABASES, CHEMICAL COMPOSITION, SELECTED PHASES *****
*****
  
```

```

if (matcalc_version<6000000)
  open-thermodyn-database mc_sample_fe2.tdb      $ Open thermodynamic database mc_sample_fe2.tdb
else
  test-exist-td-database mc_fe.tdb
  if(test_result==1)
    open-thermodyn-database mc_fe.tdb          $ Open thermodynamic database mc_fe.tdb
  
```

```

else
    send-dialog-string ""mc_fe.tdb"-database not found. Please, download it from MatCalc Website"
endif
endif
endif

```

\$ Select Fe and C as components of the system. VA (vacancies) is not necessary

```
select-elements FE C
```

\$ Select the phases which will be used in the simulation

```
select-phases FCC_A1
```

\$ Read data for the selected phases and elements from the database

```
read-thermodyn-database
```

```
read-mobility-database mc_fe.ddb
```

\$ Define the variables that will specify the initial carbon content in the bar and the thin layer

```
set-variable-value c_comp_bar_wp 1e-10
```

```
set-variable-value c_comp_layer_wp 0.8
```

\$ In the cell simulation, compositions must be entered in molar notation un\$c

```
enter-composition wp c=c_comp_bar_wp          $ Enter composition in weight percent
```

```
set-variable-value c_comp_bar un$c           $ Save the composition in mole fraction
```

```
enter-composition wp c=c_comp_layer_wp        $ Enter composition in weight percent
```

```
set-variable-value c_comp_layer un$c          $ Save the composition in mole fraction
```

```
$$*****
```

EQUILIBRIUM CALCULATIONS

```
*****$$
```

```
set-temperature-celsius 1000          $ Set the system temperature to 1000C
```

\$ Set the start values - this should prevent from any troubles in the equilibrium calculation

```
set-automatic-startvalues
```

```
calculate-equilibrium          $ Perform the equilibrium calculation
```

```
$$*****
```

PRECIPITATION DOMAIN SETUP

```
*****$$
```

```
create-precipitation-domain aus_domain      $ Create precipitation domain
```

```
set-precipitation-parameter aus_domain X FCC_A1  $ Matri[x] phase with fcc structure
```

```
$$*****
```

SIMULATION GRID

```
*****$$
```

```
use-module simulation          $ Select simulation module for cell simulation
```

```
set-variable-value num_cells_x 99          $ Define a variable representing the number of cells
```

\$ Create a simulation grid

```
create-simulation-grid num_cells_x 1 1      $ Number of cells in x-, y- and z-directions
```

```
set-variable-value barlength 0.099         $ Define a variable representing the length of the bar
```

```
set-grid-coordinates barlength 1 1         $ Dimensions in x-, y- and z-directions (in m)
```

```
set-grid-geometry p                  $ Geometry: [p]lanar, [c]ylindrical, [s]pherical
```

```
new-gui-window g5                  $ Create a new window - 2D cells
```

```
set-variable-value paint_window_id active_frame_id  $ Internal variable refers to the most actual frame
```

\$ Modify position, size and zoom level

```
move-gui-window paint_window_id 0 50 750 160  $ change position and size
```

```
set-gui-window-property paint_window_id i Z 200  $ zoom 200%
```

```
$$*****
```

CELL PROPERTIES

*****\$\$

```
create-material aus_material          $ Create material for diffusion simulation
set-material-property aus_material G D aus_domain    $ [g]eneral properties: [d]omain
set-cell-property a m aus_material      $ [a]ll cells, [m]aterial

set-variable-value diffCoeff 1e-12        $ Set the diffusion coefficient - user-specified value
set-material-property aus_material D C C F diffCoeff  $ [d]iffusion [c]oefficient of [c]arbon, [f]unction or expression

set-simulation-parameter N Y              $ Temperature i[n] celsius [y]es
set-variable-value sim_temp 1000          $ Define a variable representing the simulation temperature
$ Attach temperature to all cells
set-cell-property a V T sim_temp          $ [a]ll cells, [v]ariable, [t]emperature
$ Assign the lower carbon content, c_comp_bar, to all cells
set-cell-property a V C C c_comp_bar      $ [a]ll cells, [v]ariable, [c]omposition [c]arbon

$ Select the cell in the middle - note: first cell has index 0
set-variable-value max_cell_index num_cells_x-1
set-variable-value middle_cell_index max_cell_index/2
add-cell-selection E middle_cell_index    $ Select the c[e]ll in the centre
$ Assign the higher carbon content, c_comp_layer, to the selected cell
set-cell-property * V C C c_comp_layer
```

\$\$\$*****

GRAPHICAL DISPLAY

*****\$\$

```
$ display cell variable
set-gui-window-property paint_window_id I W V      $ S[i]mulation results, display [w]hat, [v]ariable
set-gui-window-property paint_window_id I V _cwp$c $ [v]ariable is specified
set-gui-window-property paint_window_id I R 0..1    $ [r]ange is specified
```

```
new-gui-window g1          $ Create new window: plot grid - 1D profile
$ Assign a name to both the plot window and the plot itself
set-variable-value profile_window_id active_frame_id
set-variable-value profile_plot_id last_plot_id
```

```
set-plot-option profile_plot_id S N S _cwp$c      $ Add a [s]eries, [n]ew of the [s]imulation variable
set-gui-window-property profile_window_id S U Y    $ Use default x-axis
set-gui-window-property profile_window_id S T Position [m]    $ x-axis title
set-plot-option profile_plot_id A Y 1 T Carbon content [wt.%]    $ y-axis title
set-plot-option profile_plot_id A Y 1 S 0..c_comp_layer_wp    $ y-axis range
set-plot-option profile_plot_id S M 0 numerical    $ Name the plotted series
$ Specify the range of cells
set-gui-window-property profile_window_id I t 0    $ s[t]arting cell (here 0)
set-gui-window-property profile_window_id I o max_cell_index    $ st[o]p cell (here max_cell_index)
```

```
move-gui-window profile_window_id 0 250 400 600
```

```
new-gui-window g2          $ Create new window: plot grid - cell history
$ Assign a name to both the plot window and the plot itself
set-variable-value history_window_id active_frame_id
set-variable-value history_plot_id last_plot_id
```

```
set-gui-window-property history_window_id S U Y    $ Use default x-axis
set-gui-window-property history_window_id S T Time [s]    $ x-axis title
set-gui-window-property history_window_id S S 0..sim_time    $ x-axis range
set-plot-option history_plot_id A Y 1 T Carbon content [wt.%]    $ y-axis title
set-plot-option history_plot_id A Y 1 S 0..c_comp_layer_wp    $ y-axis range
$ Add two series
```



```
set-plot-option history_plot_id S N S _cwp${middle_cell_index}    $ add composition of the middle cell
set-plot-option history_plot_id S N S _cwp${middle_cell_index-1}  $ add composition of the cell adjacent to the middle cell
$ Name the plotted series
set-plot-option history_plot_id S M 0 centre
set-plot-option history_plot_id S M 1 'next to centre'
```

```
move-gui-window history_window_id 400 250 400 600
```

```
$$*****
ANALYTICAL SOLUTION
*****$$
```

```
set-variable-value Bval c_comp_layer_wp*(barlength/num_cells_x)
set-function-expression term_1 1/(2*sqrt(pi*diffCoeff*_ctime))
set-variable-value midpt barlength/2
set-function-expression x_shifted _ccenter_x-midpt
set-function-expression term_2 exp((-1*x_shifted**2)/(4*diffCoeff*_ctime))
set-function-expression analytical_expr Bval*term_1*term_2
$ Plot series onto the existing profile plot
set-plot-option profile_plot_id S N F analytical_expr 0..barlength
```

```
$$*****
SET UP AND RUN THE SIMULATION
*****$$
```

```
$ Specify the simulation time
set-variable-value sim_time 1e7
set-simulation-parameter e sim_time          $ end
set-simulation-parameter u 10                 $ update interval
set-simulation-parameter d f                  $ diffusion-field simulation
set-simulation-parameter t i sim_temp         $ temperature: isothermal
set-default-boundary-cond G O                 $ boundary condition: [g]eometric and [o]pen to environment

start-cell-simulation

update-gui-window window-id=4
```