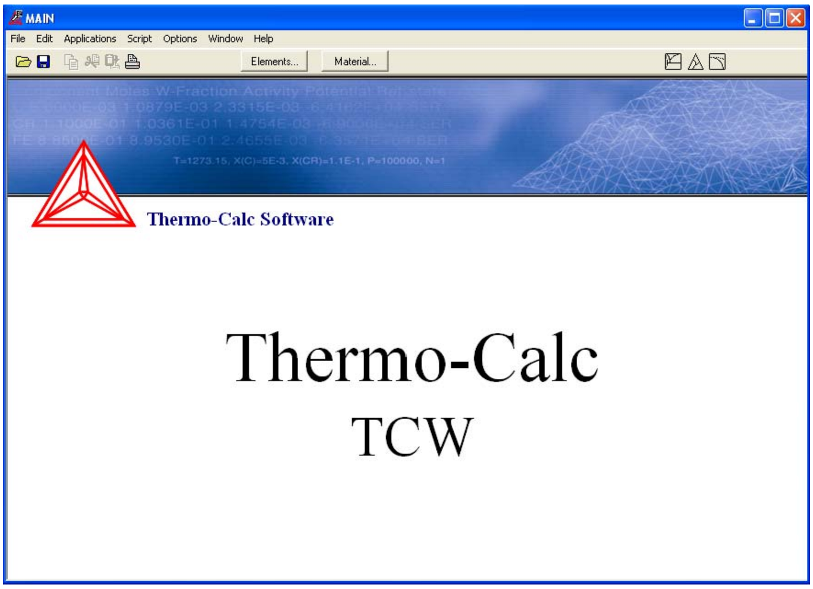
Thermo-Calc

Thermodynamics at your fingertips

1 Introduction

Thermo-Calc is the user friendly version for Windows (TCW) of the general and flexible software Thermo-Calc Classic. Thermo-Calc is designed to make advanced thermodynamic calculations easy and accessible for new, occasional and advanced users. Thermo-Calc has a graphical user interface where calculations of e.g. multicomponent phase diagrams and property diagrams, can be performed by using menus, buttons and entering a few values *e.g.* compositions. Thermo-Calc uses the same thermodynamic databases and the same calculation engine as the Classic version of Thermo-Calc software. Thermo-Calc features its user-friendliness without loss of flexibilities as emphasized in the Classic version. Thermo-Calc also features an unique advanced graphic editing facility and a Materials Organiser.



The Main Window

2 Applications

Combining an intuitive graphical user interface with a powerful engine for thermodynamic calculation, Thermo-Calc can be applied easily to perform many calculations of interest in materials science and engineering:

- Phase diagrams (binary, ternary, isothermal, isoplethal, *etc.*) *(up to 3 independent variables)*
- Thermodynamic properties of pure substances, compounds and solution phases
- Property diagrams (fraction of phases, Gibbs energy, enthalpy, C_p, volume, *etc*.) *(up to 20 components)*
- Partial gaseous pressures, chemical potentials of volatile species (up to 1000 species)
- Scheil-Gulliver solidification simulation and its extension by considering interstitial back diffusion in solid phases
- Liquidus surfaces for multicomponent alloys
- Thermodynamic factors, driving forces
- Heterogeneous equilibria *(up to 20 components)*
- Metastable equilibria
- Special quantities: *e.g.,* T_o, A_3-temperature, adiabatic T, chill factors, $\partial T/\partial X$, *etc.*
- Oxide-layer formation on steel surfaces, steel/alloy refining, so-called PRE numbers
- Evolution of hydrothermal, metamorphic, volcanic, sedimentary, weathering processes
- Speciation in corrosion, recycling, remelting, sintering, incineration, combustion
- CVD diagrams, thin-film formation
- CVM calculations, chemical ordering-disordering
- *"Anything you can think of which represents an equilibrium ..."*

3 Databases

Thermo-Calc uses the same thermodynamic databases as the Classic version. The thermodynamic databases are created by critical assessments of experimental data. Today there are accurate thermodynamic data available for many different types of materials such as:

- Steels
- Titanium alloys
- Slag
- Nickel alloys
- Minerals
- Salts
- Aluminium alloys
- Nuclear materials
- Aqueous solutions

For detailed and actual information regarding available databases see our website www.thermocalc.com.

4 Output Facilities

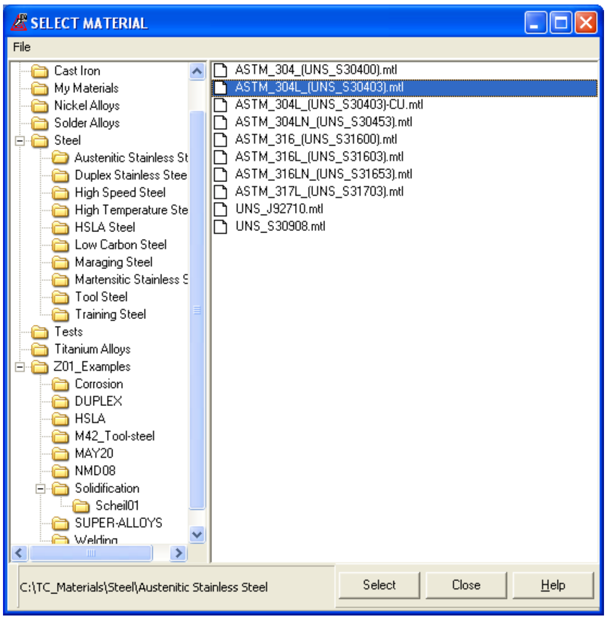
The diagrams produced in Thermo-Calc can be printed directly or saved as a graphical file in several different formats, such as Portable Networks Graphics (.png), Windows Enhanced Meta Format (.emf), Acrobat (.pdf), JPEG (.jpg), TIFF (.tif), Post Script (.ps), etc. With all these formats available it is easy to incorporate your figures into a written report. The Windows Enhanced Meta Format also gives the user the possibility to incorporate and edit diagrams in reports and presentations. Thermo-Calc allows the user to tabulate a property diagram and export it to Microsoft Excel. With this recent development it is possible to use the functionality in Microsoft Excel to tabulate and plot thermodynamic functions and properties calculated by Thermo-Calc.

5 Availability

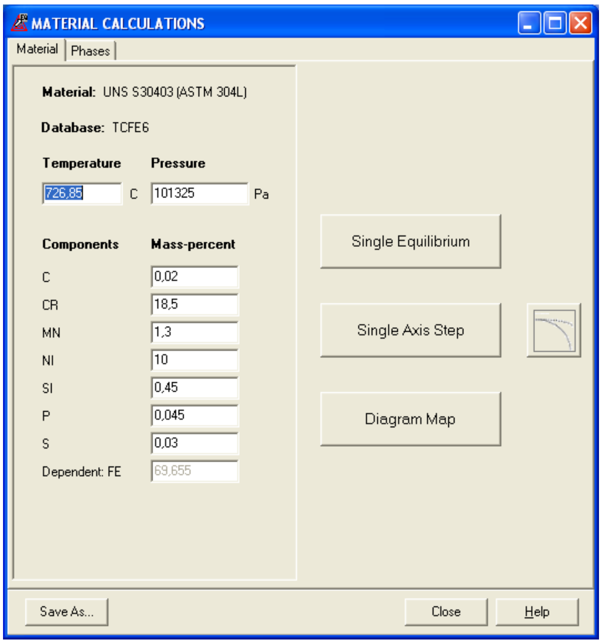
Thermo-Calc is at present available for PC/Windows environment only with the O/S Windows Vista Business and XP.

6 Calculation Example 1

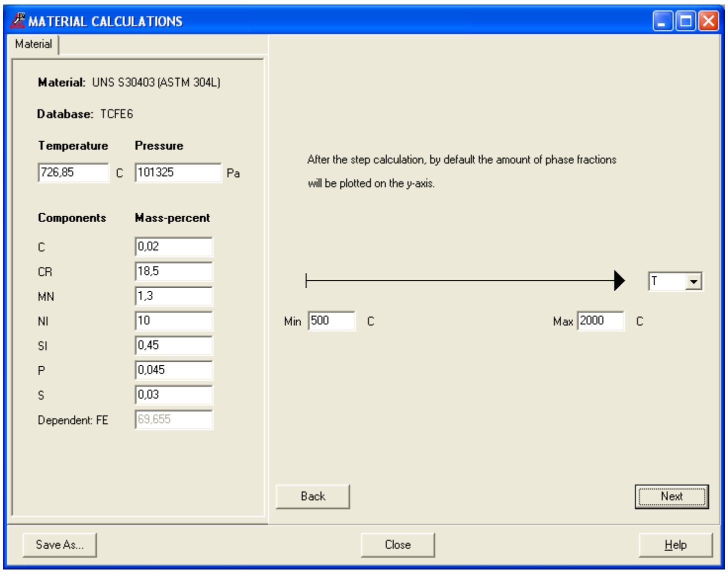
The example below shows one of the simple ways to calculate phase fractions and phase compositions for an austenitic stainless steel as a function of temperature. Open the Materials Organiser and select, edit or add a new material.



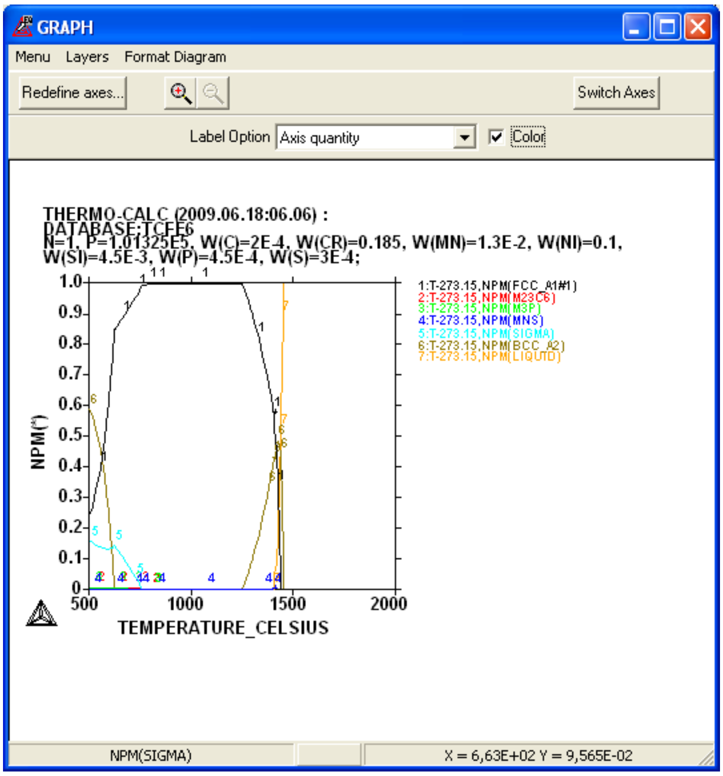
Check your composition and conditions. Select computation method. For phase fractions and phase compositions we select Single Axis Step.



Select the Temperature interval you want to run your computation for

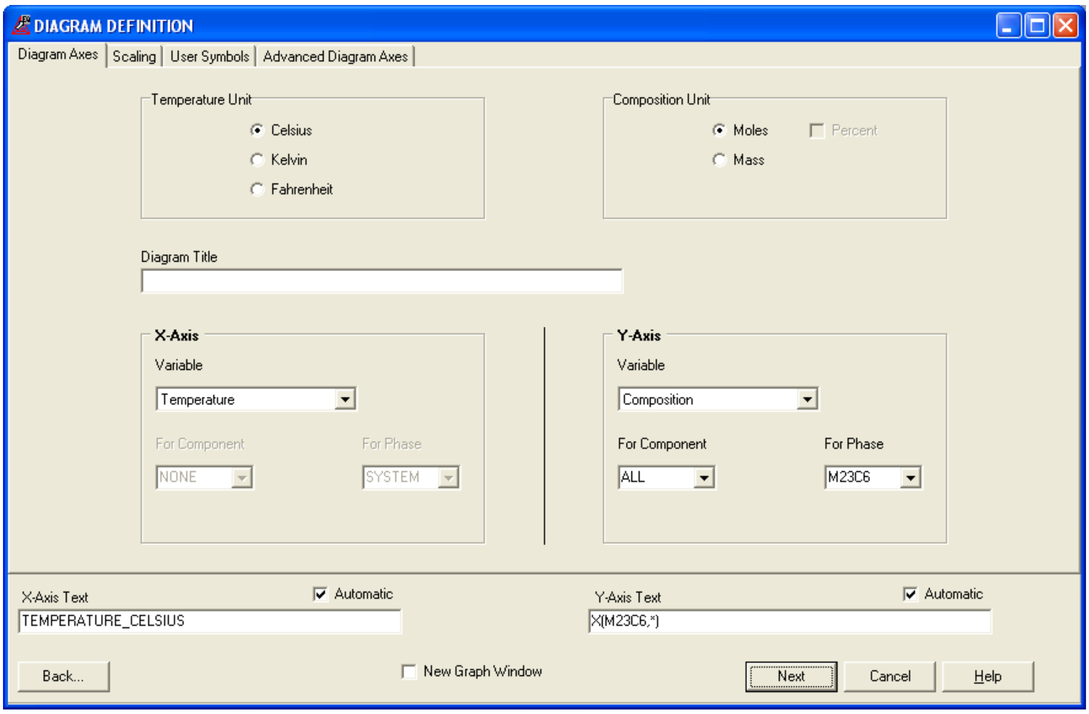


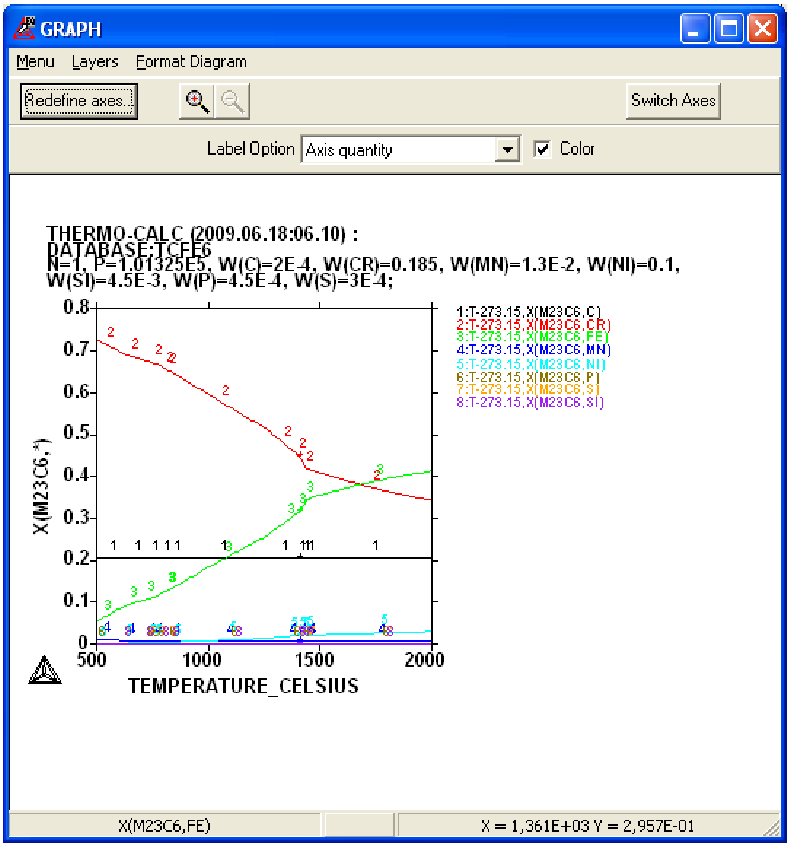
Click next and Thermo-Calc will perform the computation and generate the plot.



In the plot window you can analyse the graphic results by moving the cursor over the plot areas, lines etc., and read off the coordinates, phase information in the bottom to the left and right.

You can also Redefine the axis and make many different plots based on the same computation e.g. redefine the y-axis to *Composition* and select a phase for example M23C6 to investigate the phase composition..



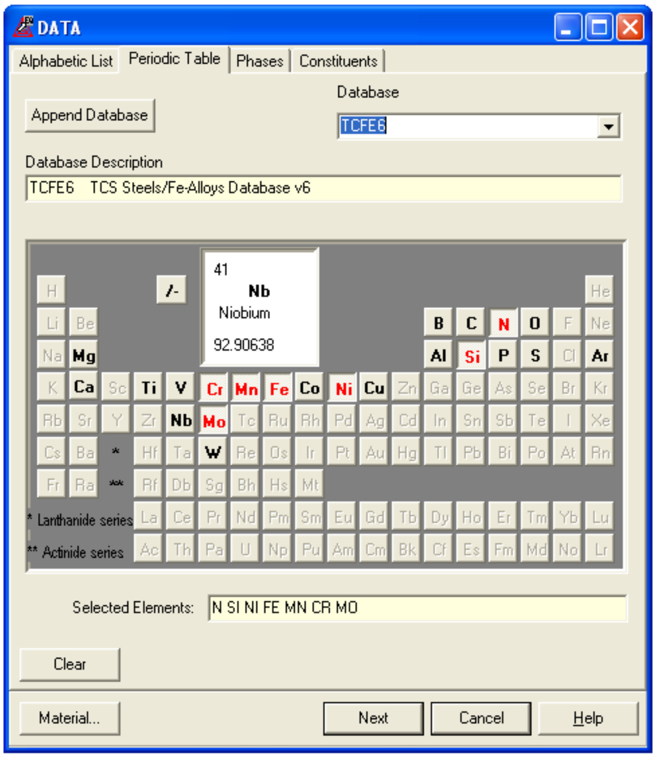


You can continue the graphic analysis of the results and you can continue to redefine the plots for more phases, specific elements and other properties in many different ways without the need of a new calculation.

You can of course save your result in different formats and you can easily start a new computation with the same materials composition as a base with the possibility to change the composition or add/remove elements. The effects of such changes can quickly be investigated with Thermo-Calc and the use of the Materials Organiser.

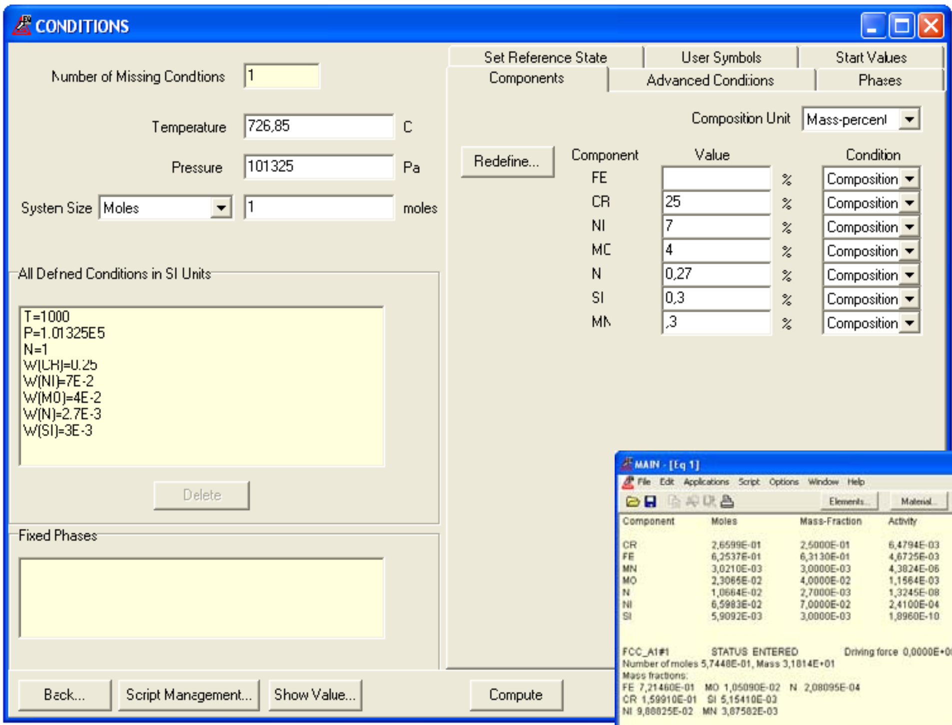
7 Calculation Example 2

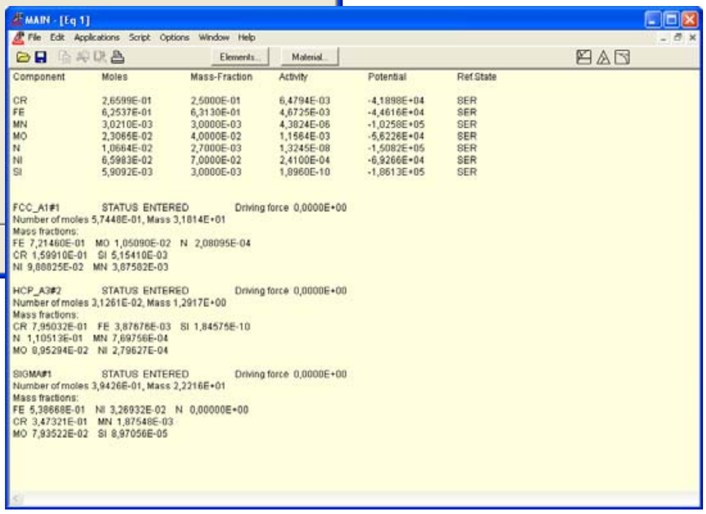
The example below shows the classic method to calculate phase fractions and phase compositions as a function of temperature for a duplex stainless steel with the user friendly interface.



The composition of the steel is Fe-25Cr-7Ni-4Mo-0.27N-0.3Si-0.3Mn (wt%) and the phase fractions and compositions will be calculated in the temperature interval 873 to 1773 K.

Open the Thermo-Calc program and click the *Elements…* button in the MAIN window, the DATA window is then launched. Select the thermodynamic database and elements to be used in the calculation. Click the *Next* button, the CONDITIONS window appears.

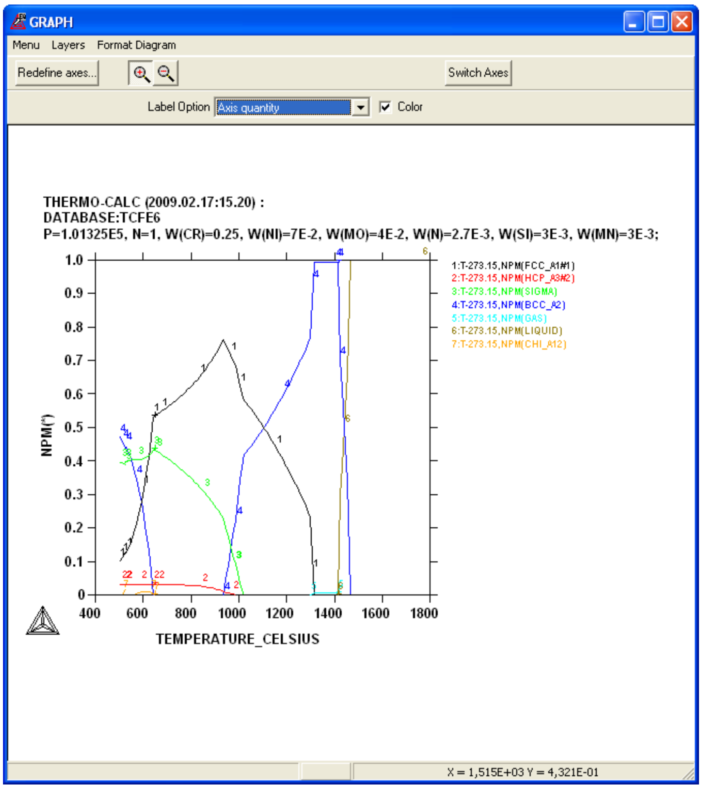




Specify the composition (Fe-25Cr-7Ni-4Mo-0.27N-0.3Si-0.3Mn in wt%), initial temperature (1373 K), system size (1 mole) and pressure (100000 Pa). Click *Next*, the phase equilibrium at the specified conditions is then calculated. We find that the equilibrium state, listed in the MAIN window, is a mixture of ferrite (BCC_A2#1) and austenite (FCC_A1#1).

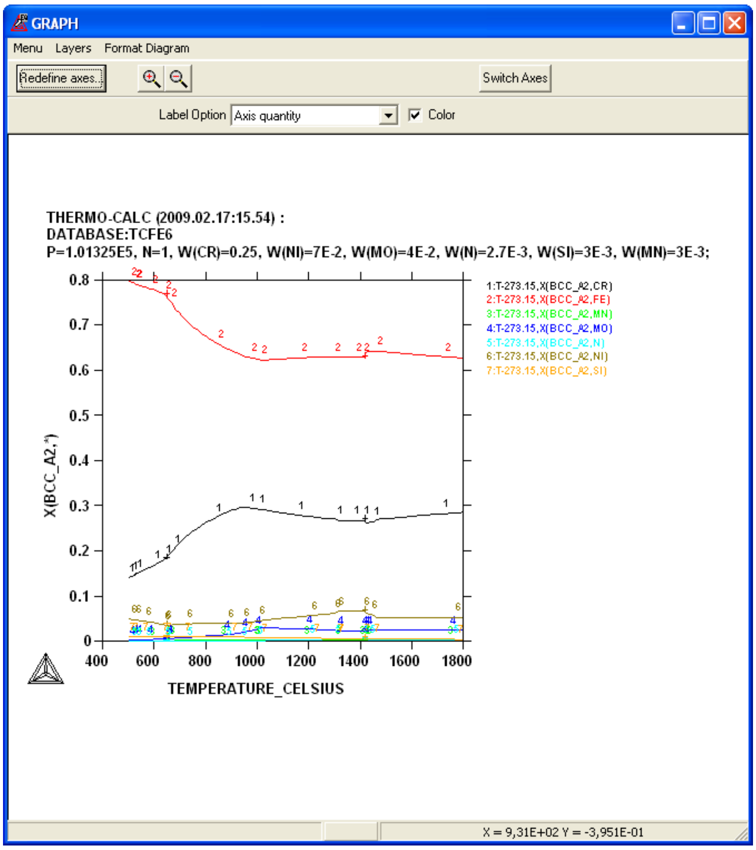
The compositions of the phases are also listed. Meanwhile, the MAP/STEP DEFINITION window pops up. After choosing temperature as the only independently-varying variable, click the *Next* button; phase equilibrium at different temperatures will be calculated and many different types of diagrams can then be plotted from this calculation by defining various variables as axes in the DIAGRAM DEFINITION window, where temperature and phase fraction will appear as the default plotting axes.

Simply accept the default axes and plot this property diagram by clicking *Next*. The obtained diagram shows where there is a risk for forming secondary phases such as Cr2N (HCP_A3#2) and sigma phase, which have a detrimental effect on the material properties.



From the same calculation, many more diagrams can be plotted. Using the *Redefine* button, one can plot for example the variation of the composition of the ferrite phase with temperature.

As we can see from this diagram, at temperatures below 1280 K the content of chromium and molybdenum decreases since secondary phases such as sigma phase and Cr_2N are stable in this temperature region.



One quick calculation provides lots of useful information.