
Introduction to OpenCalphad

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FH-Wels

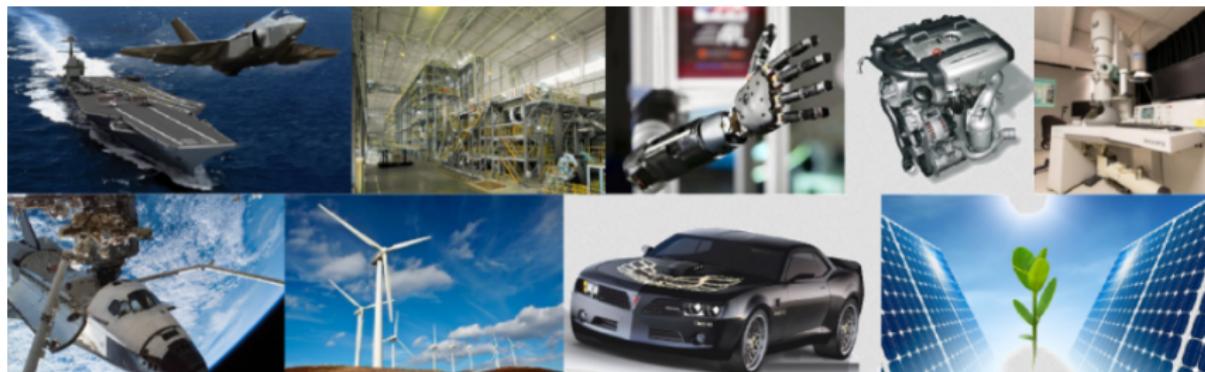
MSDM 2021, Tue. July 13th

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1. Introduction

- Metals sciences
 - Materials play today an important role in the industry
 - Interdisciplinary field of study
 - Metals are ideally suited for many sectors and applications, and as well for high-tech designs



1. Introduction

• Applications

- Possible requirements: new alloys, improved mechanical properties, corrosion resistance,...



Bridges: high-strength steels



Olympiastadion Athen 2004



Marine and Offshore Applications



Steam turbines



Steam turbines



Railways

1. Introduction

- Parameters influencing the material properties
 - Chemical composition,
 - Thermodynamics, solid solutions,
 - Dislocations,
 - Strengthening mechanisms,
 - Atomistic mechanisms,
 - Microstructure, multiphase materials,
 - Phase transformation, nucleation,
 - Thermo-mechanical processing, heat-treatments.

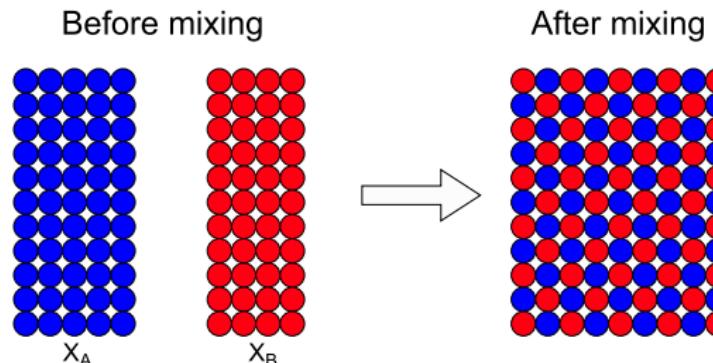
1. Introduction

- Aims

- The aim of this presentation is to give an introduction to the methods of Calphad, including the solution solution models applied for metals, using OpenCalphad
- The effect of alloying elements such as Cr, Ni, Mn, and Si on the phase diagrams was calculated
- The plots of ternary diagrams, Gibbs energy, and phase diagrams are given, which allows to give a better assessment of the possibilities of OC

2. Thermodynamics

- Description with the Gibbs-Energy
 - Example for A - B System



Free energy:

$$X_A G_A$$

Free energy:

$$X_B G_B$$

$$\text{Total free energy: } G_1 = G_A + \Delta G_{\text{mix}}$$

$$\text{Total free energy: } G_1 = X_A G_A + X_B G_B$$

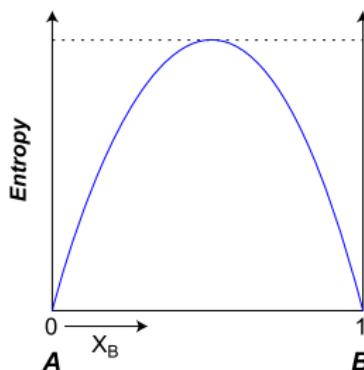
[L. Samek (C)]

2. Thermodynamics

- Description with the Gibbs-Energy for A and B

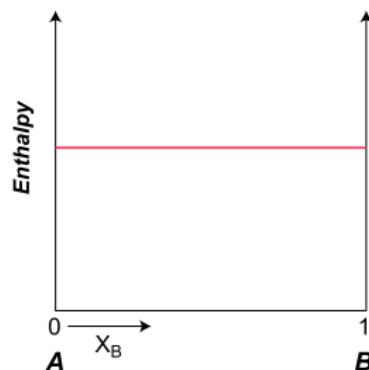
Entropy of mixing

$$\Delta S_{\text{mix}} = -R(X_A \ln X_A + X_B \ln X_B)$$



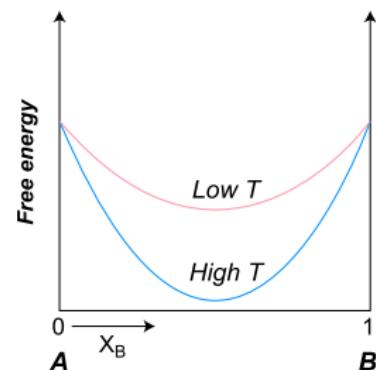
Enthalpy of mixing

$$\Delta H_{\text{mix}} = 0$$



Free energy of mixing

$$\Delta G_{\text{mix}} = -T\Delta S_{\text{mix}}$$



[L. Samek (C)]

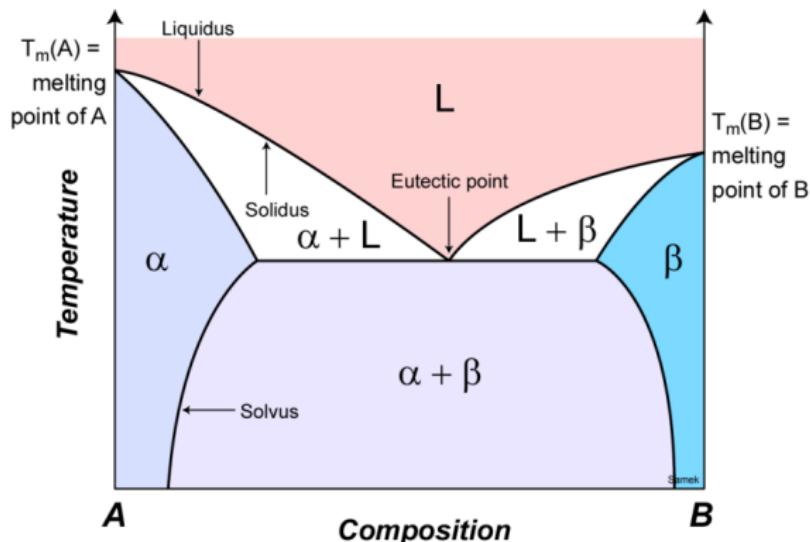
Total free energy of the ideal solid solution: $G_2 = X_A G_A + X_B G_B + \Delta G_{\text{mix}} = X_A G_A + X_B G_B + RT(X_A \ln X_A + X_B \ln X_B)$

2. Thermodynamics

- Description of the Gibbs-Energy for non ideal solutions
 - $\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix}$
 - $\Delta G_{mix} = \Omega X_A X_B + RT(X_A \ln X_A + X_B \ln X_B)$
- Reactions:
 - Exothermic process $\Delta H_{mix} < 0$
 - Endothermic process $\Delta H_{mix} > 0$

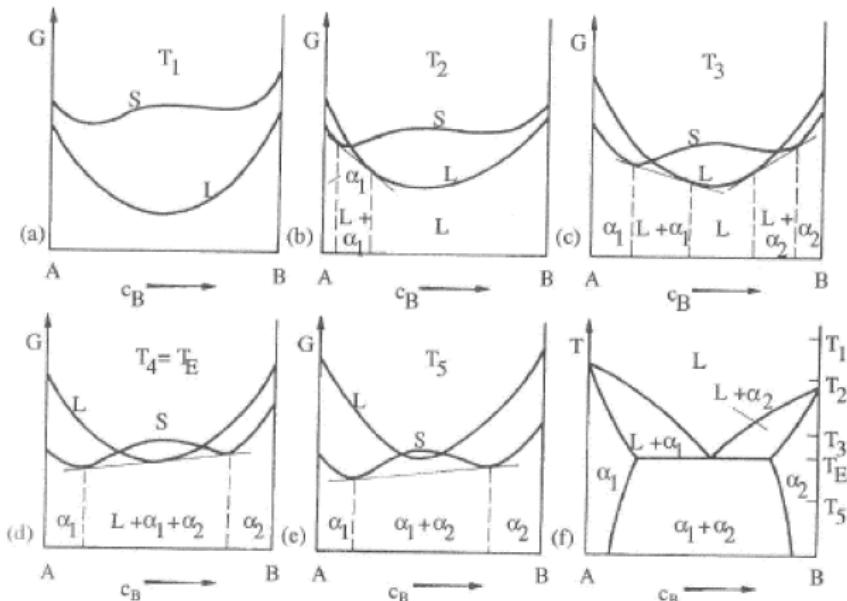
2. Thermodynamics

- Illustration for obtaining the phase diagram
 - Diagram with eutectic point, α , β , and L



2. Thermodynamics

- Relation between the Gibbs-Energy and the phase diagram



3. OpenCalphad

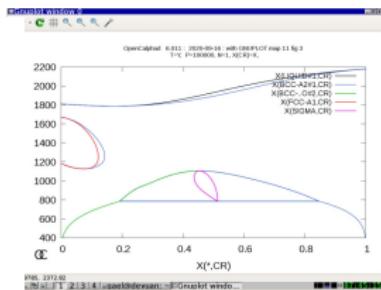
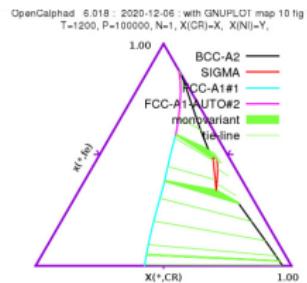
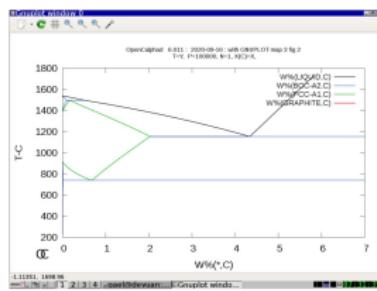
- Thermodynamic calculations
 - OpenCalphad (OC) is an international collaboration of scientists and researchers in the development of methods for thermodynamic calculations.
 - It allows to develop thermodynamic models and database for alloys.



OpenCalphad

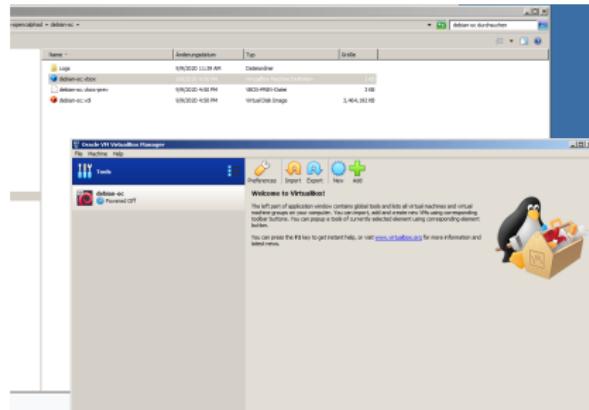
3. OpenCalphad

- Range of applications
 - Material designs, database, thermodynamics, and models,
 - Studying phase diagrams, alloy design, binary and ternary diagrams,...
 - Example of calculations using OC (binary and ternary phase diagrams):



3. OpenCalphad

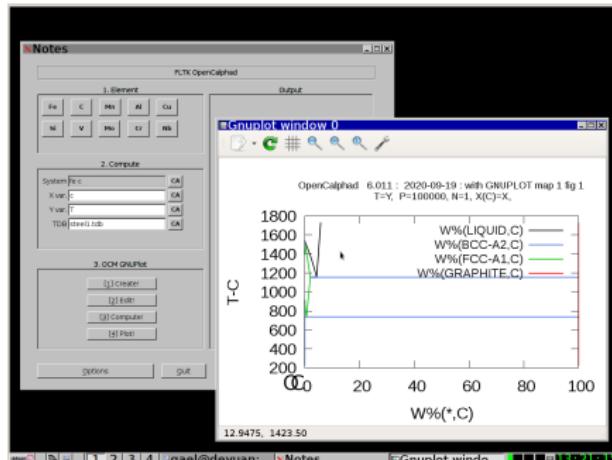
- Installation of virtual machine
 - The opensource software **VirtualBox** is installed on the machine (Win, Mac, Linux/Unix)
 - OpenCalphad is already compiled from source and installed on the virtual image



3. OpenCalphad

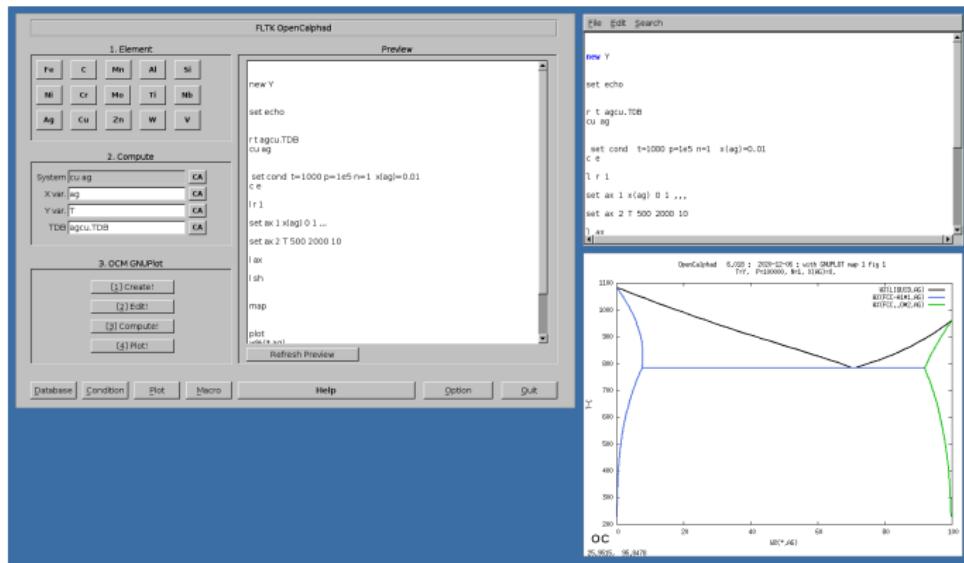
- Available user interfaces

- Terminal user interface (TUI) and graphical user interface (GUI)
- CAE OpenCalphad (non opensource) and the opensource graphical interface using the FLTK Library



4. Studying Ag-Cu system and Fe-C system

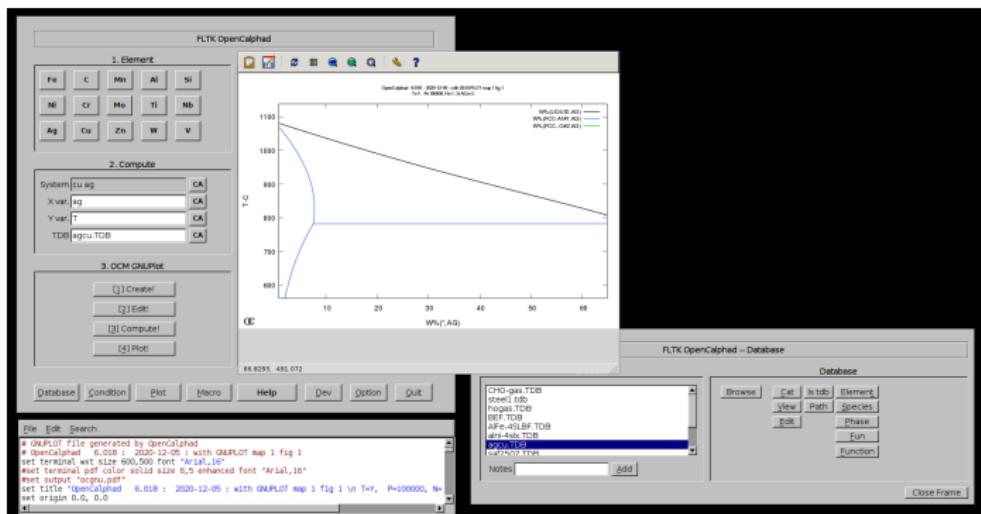
- Calculation of the phase diagram for the Ag-Cu system
 - 1.) Create, 2.) Edit, 3.) Compute, and 4.) Plot



4. Studying Ag-Cu system and Fe-C system

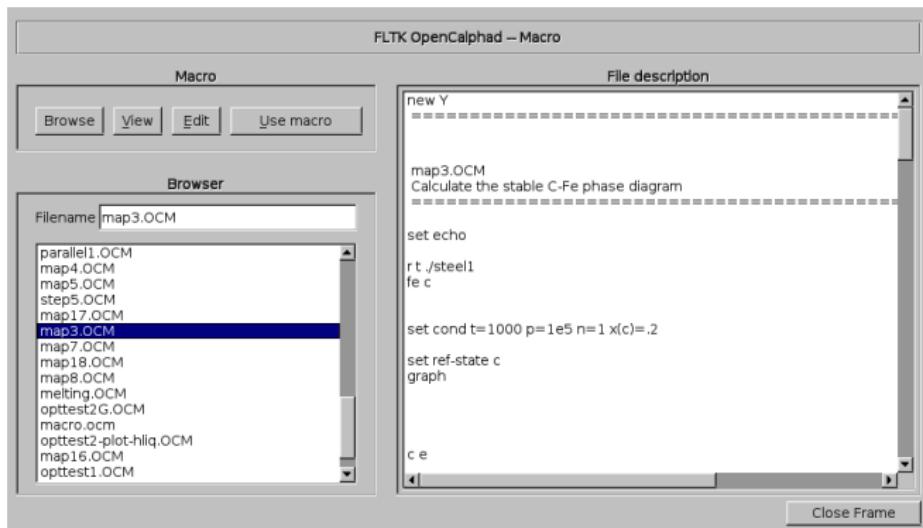
• Database

- The module "Database" allows to select a given database (TDB file)



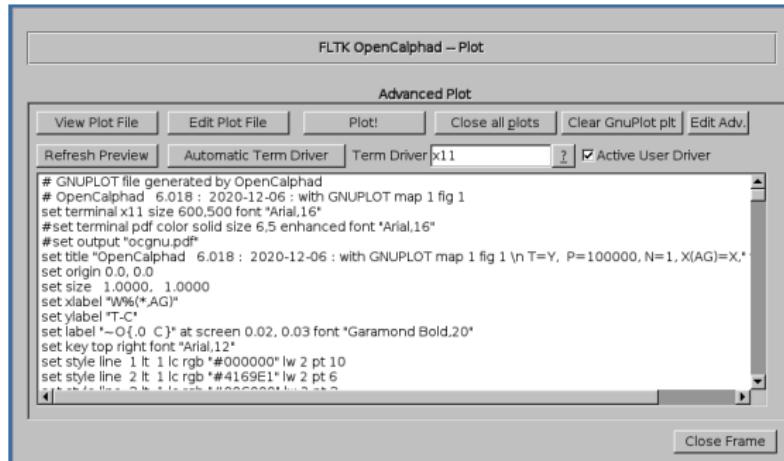
4. Studying Ag-Cu system and Fe-C system

- Interface to edit and load a "Macro" for calculations
 - It allows the researcher or student to exchange and select the calculation



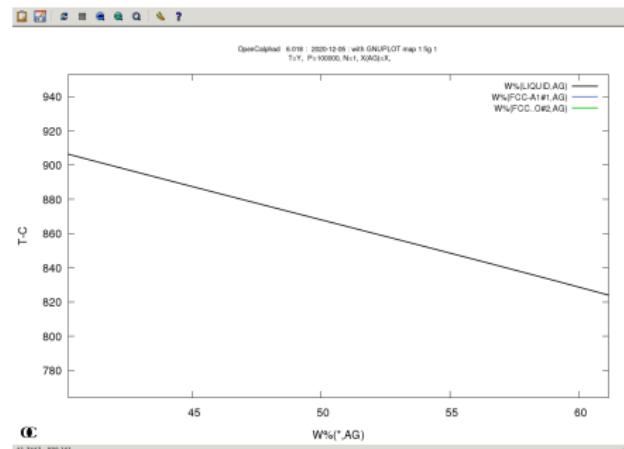
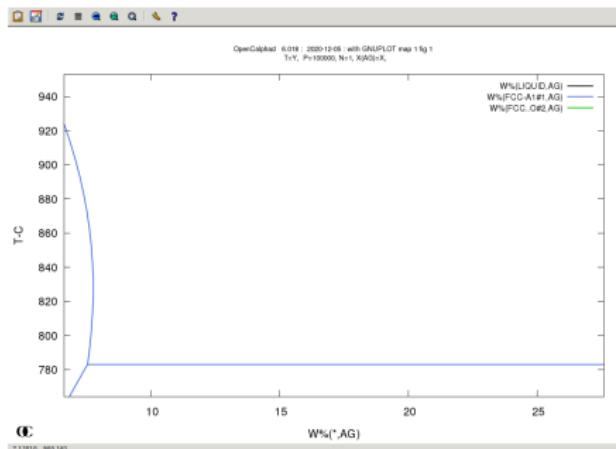
4. Studying Ag-Cu system and Fe-C system

- Advanced plot module
 - [Gnuplot](#) allows to modify and display the calculated phase diagram.
 - The user can view and edit the plot.



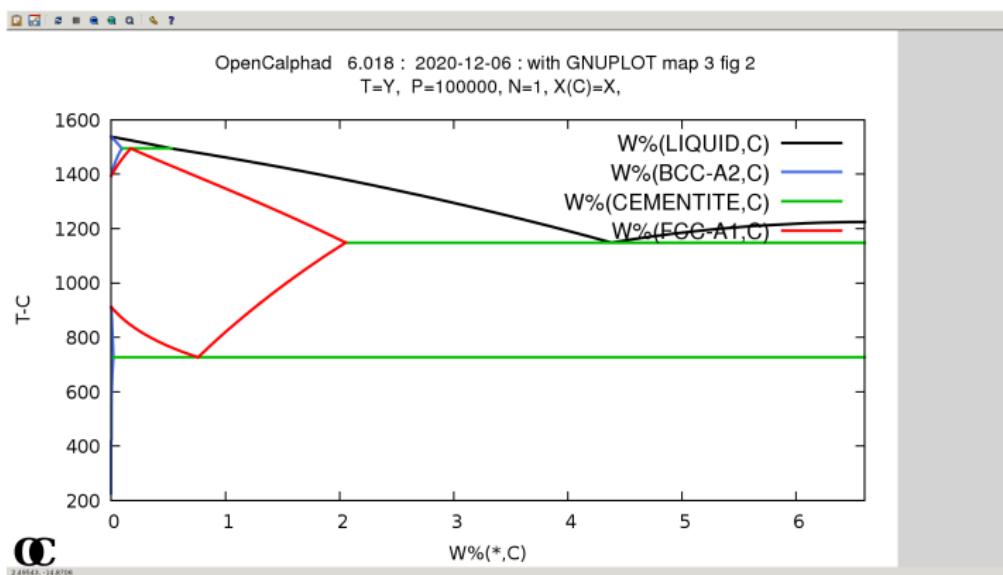
4. Studying Ag-Cu system and Fe-C system

- Functionality to study the phase diagram
 - It allows with a **zoom** to view with the cursor the coordinates
 - It allows material scientist, researcher or student **to study the phase diagram**



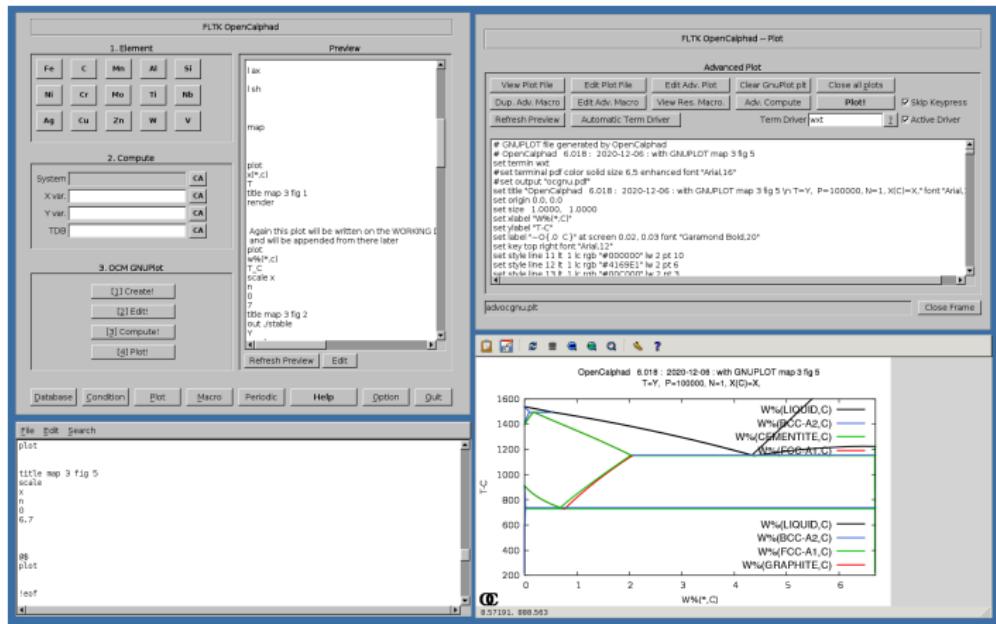
4. Studying Ag-Cu system and Fe-C system

- Calculations of the phase diagram for Fe-C, metastable
 - Allows studying the Fe-C phase diagram for education



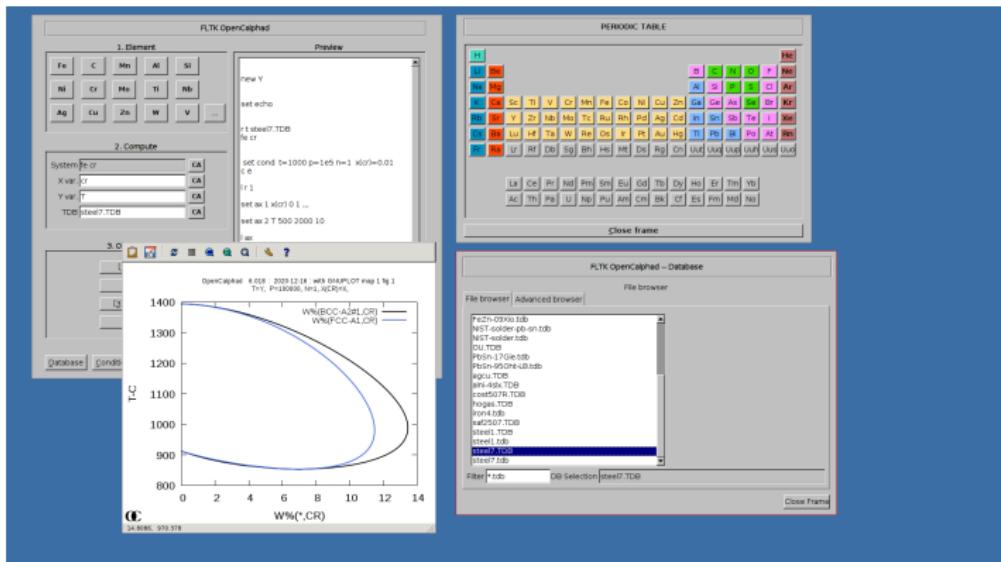
4. Studying Ag-Cu system and Fe-C system

- Metastable and stable phase diagrams



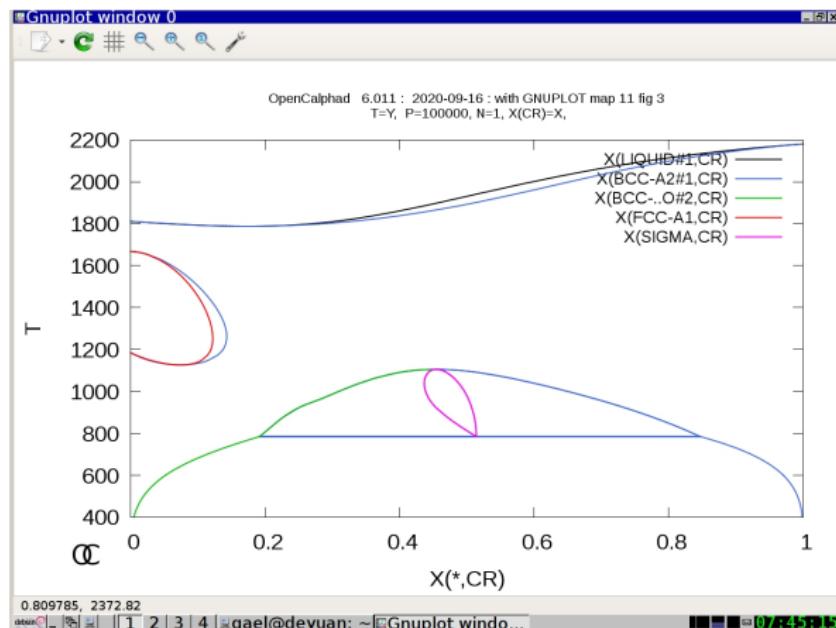
5. Fe-Cr, Fe-C-Cr and Fe-Cr-Ni systems

- Choice of elements for calculations
 - Influence of Cr (Fe-Cr system)



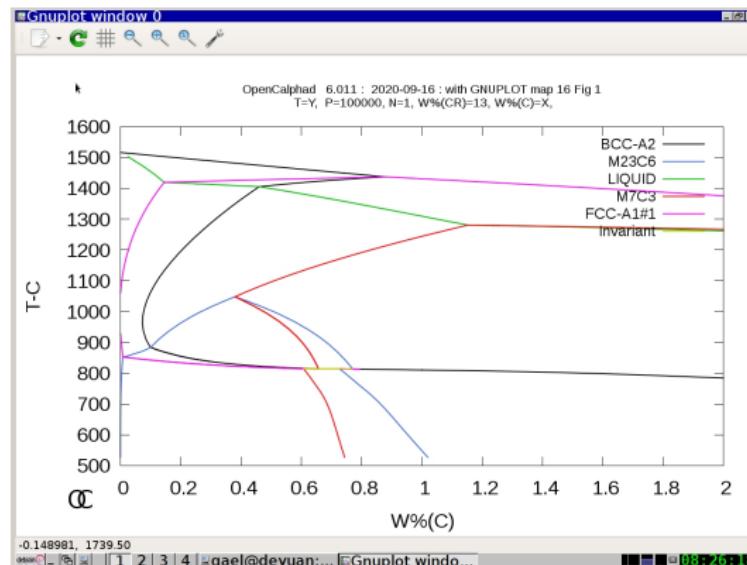
5. Fe-Cr, Fe-C-Cr and Fe-Cr-Ni systems

- Fe-Cr system



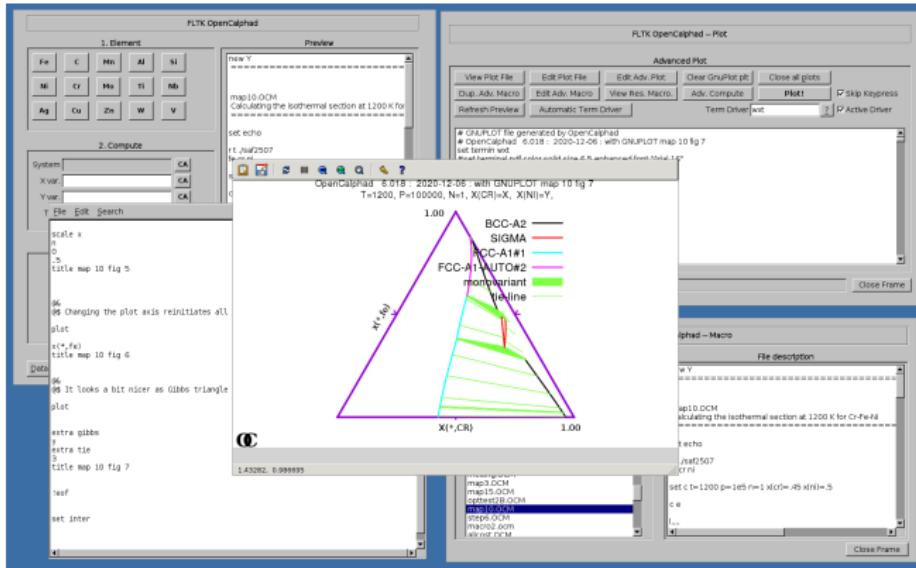
5. Fe-Cr, Fe-C-Cr and Fe-Cr-Ni systems

- Calculations with 13 wt.-%Cr for Fe-C-Cr system
 - Example for stainless steels



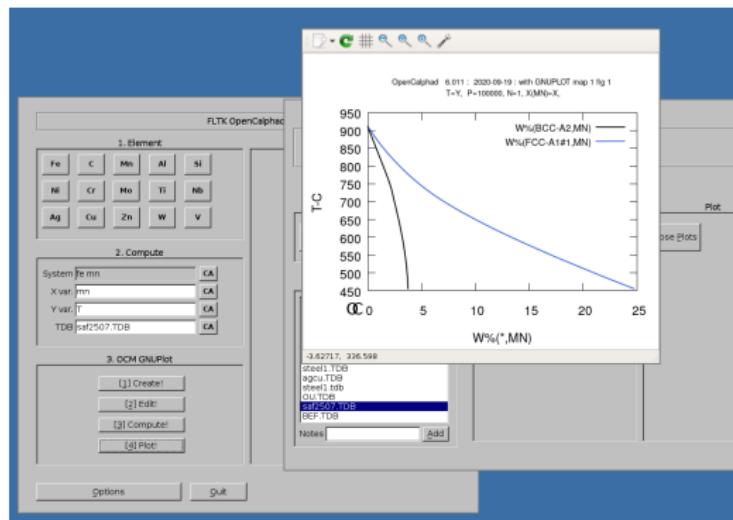
5. Fe-Cr, Fe-C-Cr and Fe-Cr-Ni systems

- Ternary phase diagram
 - Isothermal section for a given temperature for Fe-Cr-Ni system



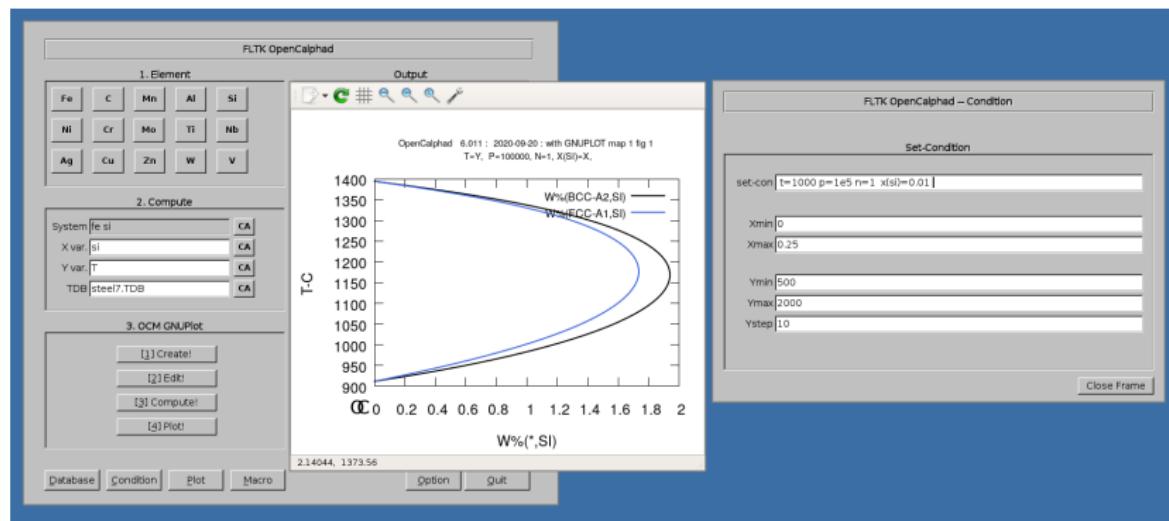
6. Calculations for modern steel design

- High-strength steels
 - Fe-Mn system
 - Influence of Mn on the phase diagram:



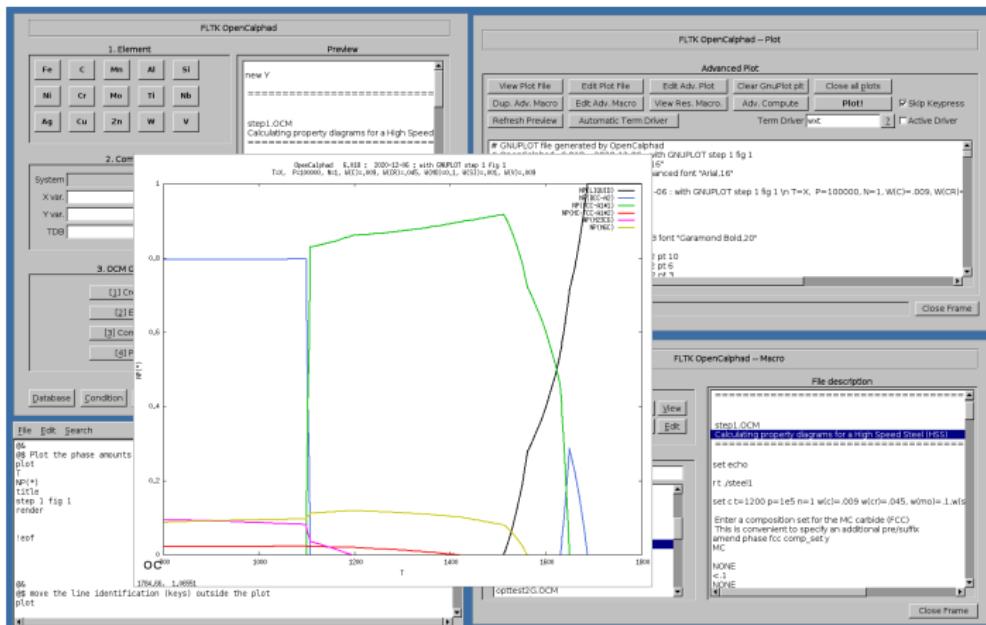
6. Calculations for modern steel design

- High-strength steels
 - Fe-Si system
 - Influence of Si on the phase diagram:



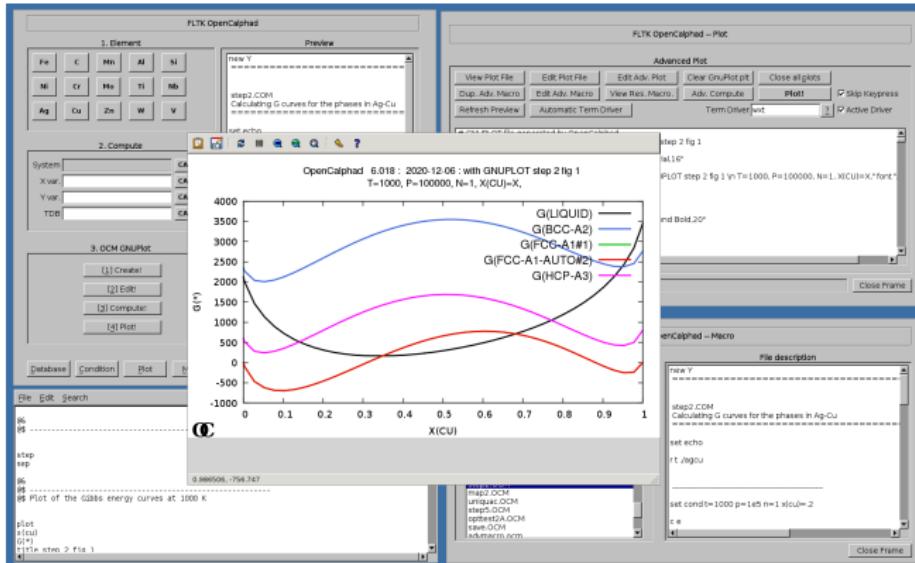
6. Calculations for modern steel design

- Results for high-speed steels



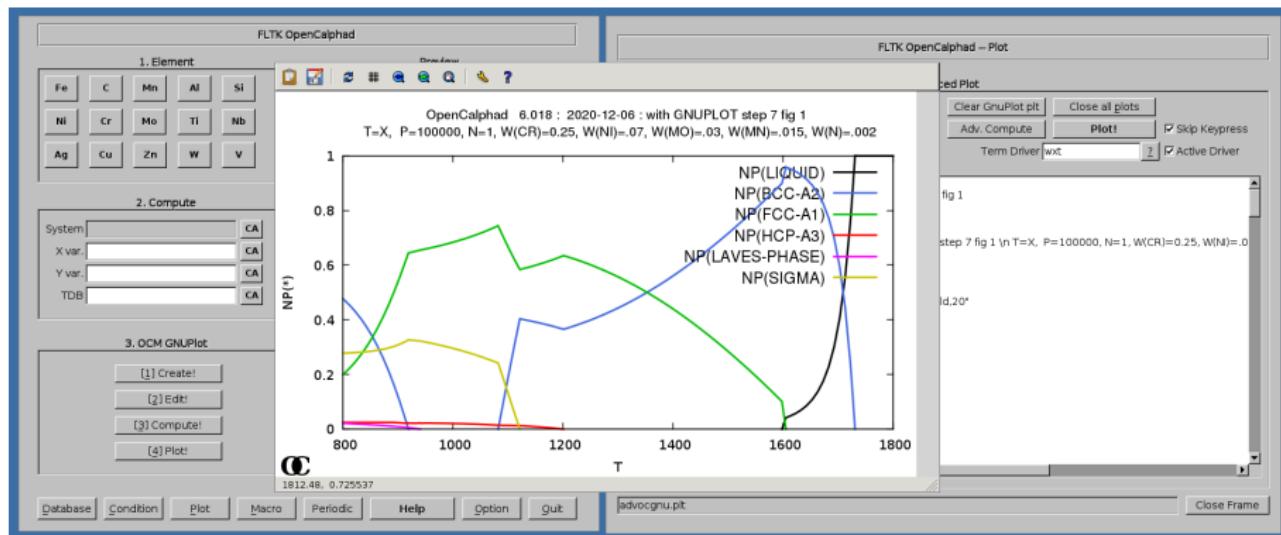
7. Advanced calculations

- Plot of user defined functions
 - Gibbs energy for Ag-Cu system



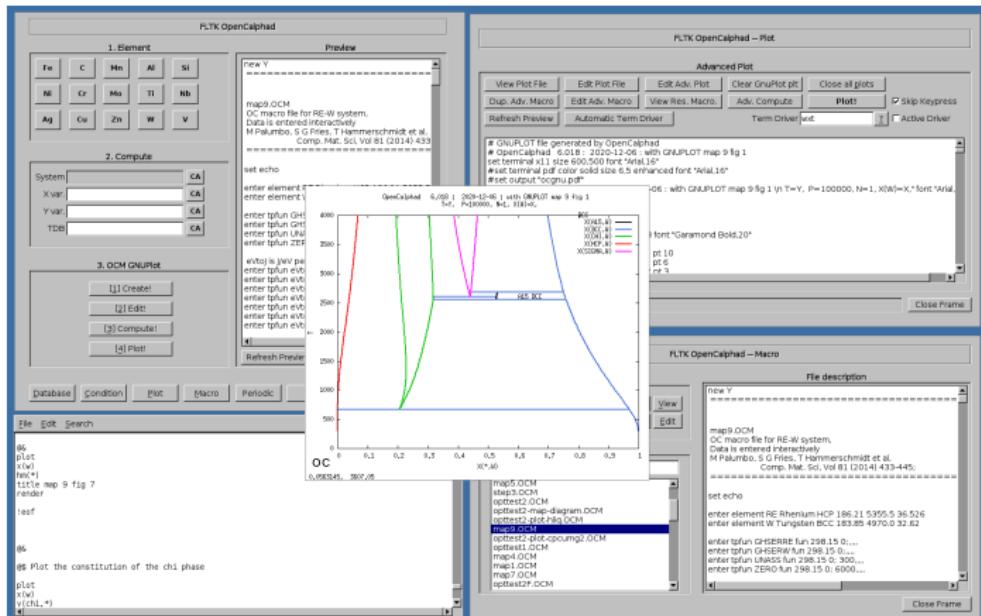
7. Advanced calculations

- Property diagrams for special alloys
 - This allows for instance to study precipitation



7. Advanced calculations

- Rhenium-Tungsten (Palumbo, Fries, Comp. Mat. Sci., 2014)



8. Conclusions

- OpenCalphad is an [opensource project](#), which is ideally suited for material scientists interested in chemistry, thermodynamics and materials science
- Unique large range of possibilities given by OC
- Possibility to [develop models and database](#)
- GUI frontend allowing [to edit and develop database for OC](#)
- It offers the possibility to develop an user community to [establish scientific exchanges](#)