

# Thermo-Calc Software

## Thermo-Calc On-line Training

Day 2 *October 8, 2025*



## Thermo-Calc Day 2

- 9:00 About the home assignment.
- 9:10 Thermodynamic Databases.
- 9:30 Step 3: Al alloy 6053
- 9:55 Map 1: Phase diagram for a cemented carbide.
- 10:25 Q & A
- 10:40 Map 2: HEA phase diagram.
- 11:05 Map 3: Phase diagram from base material to weld.
- 11:40 Q & A
- 11:55 Handing out home assignment.

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Step = One-axis Step Calculation

Map = Phase diagram mapping, 2 axes or more.

# Home assignment 1 – Fixing phase

Material: Tool Steels - Database: TCFE14 !

1) Fe-4Cr-8Mo-2V-0.3Mn-0.3Si-1C (wt-%)

- a) Calculate the liquidus temperature for the steel.
- b) How does the liquidus temperature change with carbon content?

More than one way to solve!

# Home assignment 1 - solution

At least two methods to solve this:

## 1) Graphic

- a) One-axis stepping in T and read Liquidus-T from a T vs. “Mole-fraction of phase”-diagram
- b) Phase diagram mapping, plot wt-% C vs. T

## 2) Using phase status

- a) Single-equilibrium calculation with LIQUID as FIX phase with 1 mole (in a system where  $N=1$ ).
- b) One-axis step calculation in W(C) with the same condition on the LIQUID's phase status.

Material: Tool Steels

1) Fe-4Cr-8Mo-2V-0.3Mn-0.3Si-1C

- a) What is the liquidus temperature for the steel?
  - 1684.5 K (1411°C)
- b) How does the liquidus temperature change with carbon content?
  - Decreasing with increasing carbon content in a fairly linear fashion (as long as the stable phases are the same). See next slide.

# Home assignment 1 - Results

1) Fe-4Cr-8Mo-2V-0.3Mn-0.3Si-1C

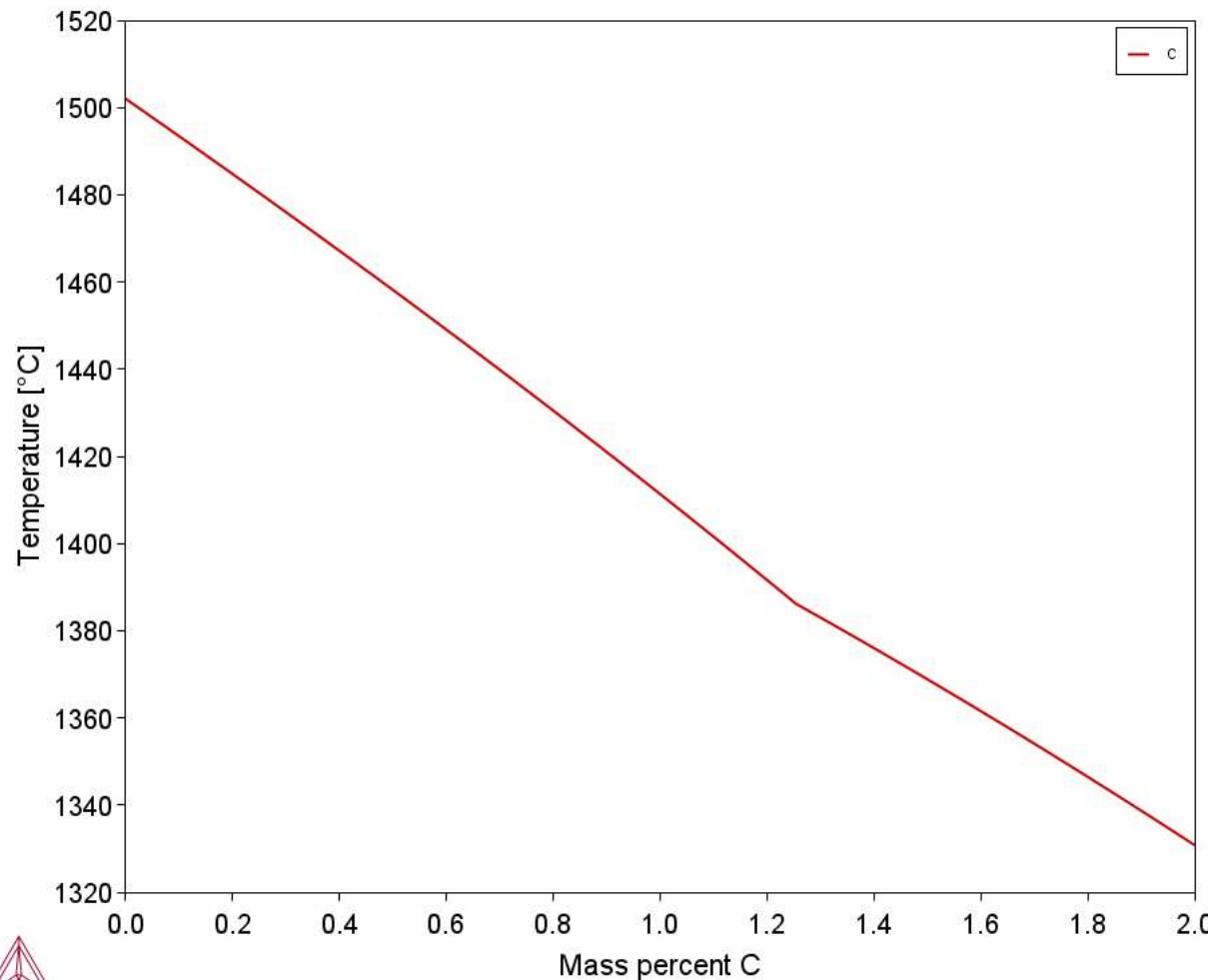
b) Step with the conditions on FIX LIQUID still on.

2025.03.27.11.43.23

TCFE14 : Fe, Cr, Mo, V, Mn, Si, C

Temperature [°C] = 1400.0, Pressure [Pa] = 100000.0, System size [mol] = 1.0, Mass percent Cr = 4.0, Mass percent Mo = 8.0, Mass percent V = 2.0, Mass percent Mn = 0.3, Mass percent Si = 0.3, Mass percent C = 1.0

Pressure [Pa] = 100000.0, System size [mol] = 1.0, Fix phase: LIQUID = 1.0, Mass percent Cr = 4.0, Mass percent Mo = 8.0, Mass percent V = 2.0, Mass percent Mn = 0.3, Mass percent Si = 0.3



# Thermodynamic Databases

A database in our understanding means *a collection of polynomials describing some property for the individual phases of a system, as a function of temperature, (pressure) and composition.*

**Databases are developed using the CALPHAD method.**

☐ Thermodynamic data  $\Rightarrow$  All our software tools

- Gibbs free energy, i.e.  $G_m^\phi = f(T, P, x_i^\phi)$

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☐ Kinetic data  $\Rightarrow$  DICTRA, TC-PRISMA

- Atomic mobility

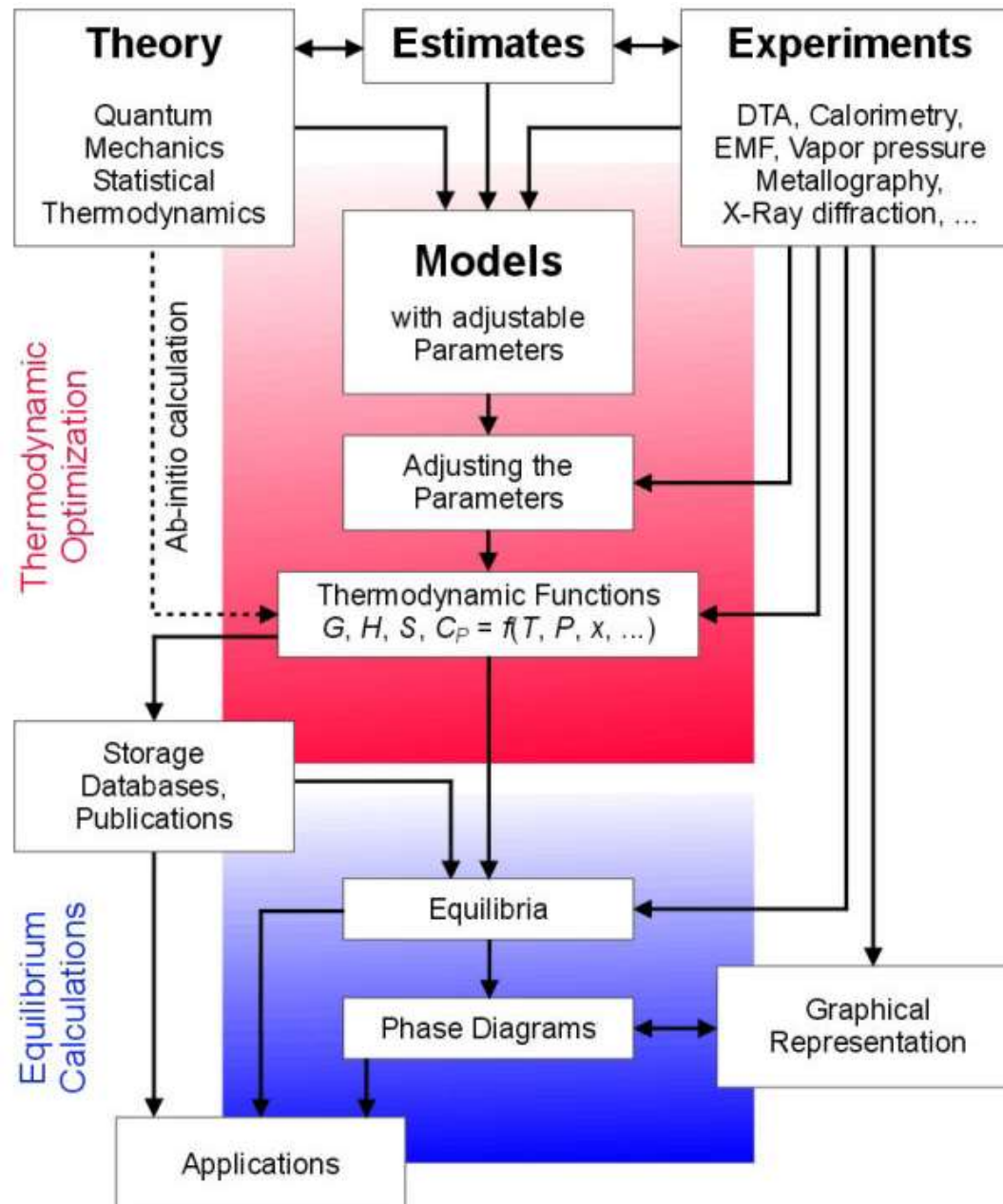
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☐ Property data

- Molar volume  $\Rightarrow$  TC, TC-PRISMA
- Interfacial energies (no database)  $\Rightarrow$  TC-PRISMA
- Thermal conductivity  $\Rightarrow$  TC
- Electric conductivity  $\Rightarrow$  TC
- Viscosity in liquid  $\Rightarrow$  TC
- Liquid surface tension  $\Rightarrow$  TC
- ....more will follow

- ☐ Unary systems.  $G=G(T)$  for all stable and metastable phases included in database.
  - ☐ Binary systems (or parts of).  $G=G(T,x)$  for stable and metastable phases, including binary phases.
  - ☐ Ternary systems (or parts of). See above.
  - ☐ Higher order systems (parts of).
- 
- ☐ Databases are produced by critical assessment of experimental data and optimization of model parameters (the CALPHAD method).
  - ☐ PARROT in Thermo-Calc Console Mode can be used as a tool in this process.

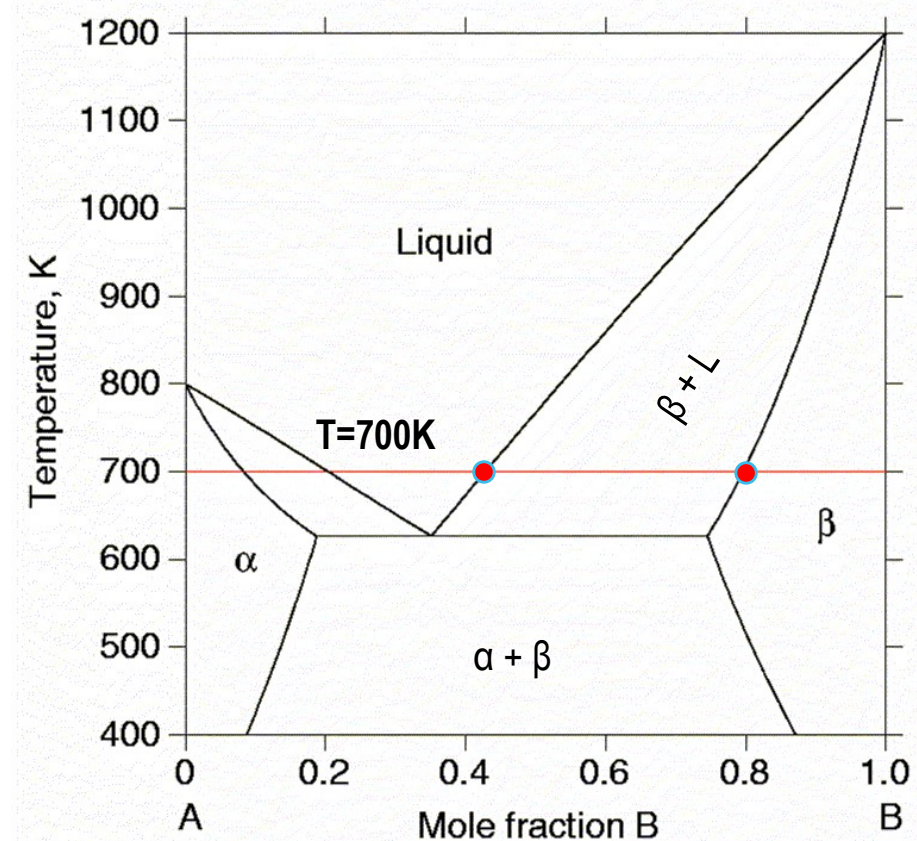
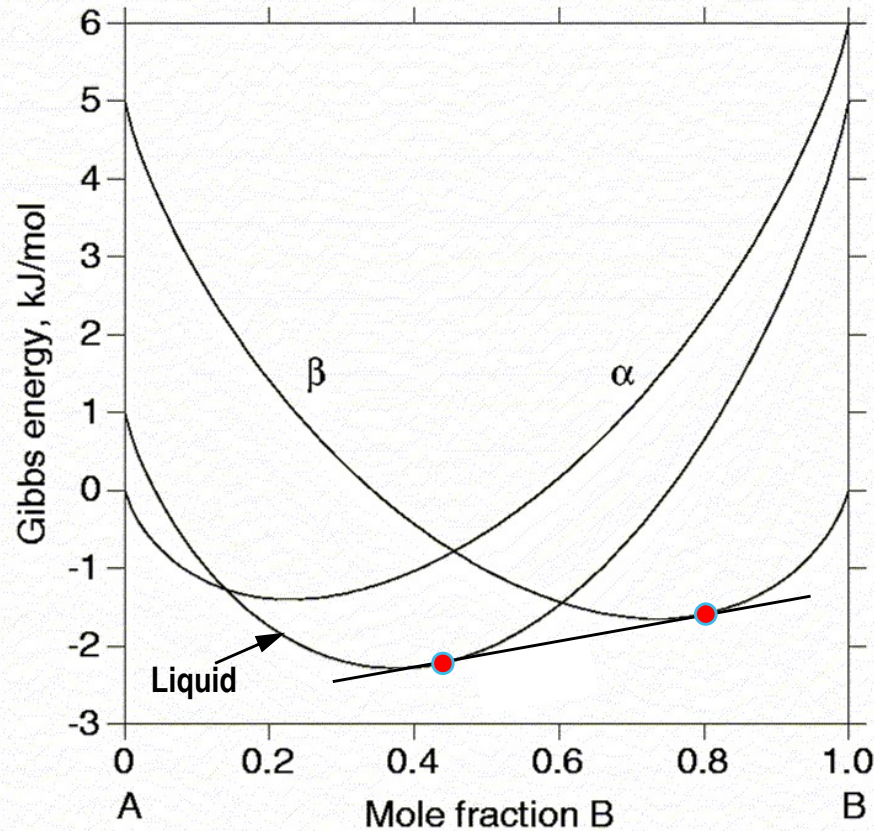
# The CALPHAD Method



# The CALPHAD Method

Originally «CALculation of PHase Diagrams»

Now: «Computer coupling of phase diagrams and thermodynamics»



$$G^{\alpha}(x)_T = x_A G^{\alpha} + x_B G^{\alpha} + RT(x_A \ln x_A + x_B \ln x_B) + x_A x_B L^E$$

$$G^{\alpha}(T)_x = A + BT + CT \ln(T) + ET^{-1} + FT^2 + \dots$$

Gibbs free energy per mole for a solution phase is normally divided in:

$$G_m = G_m^0 + \Delta G_m^{ideal} + \Delta G_m^E + \Delta G_m^{ph}$$

reference surface

configurational contribution

excess term

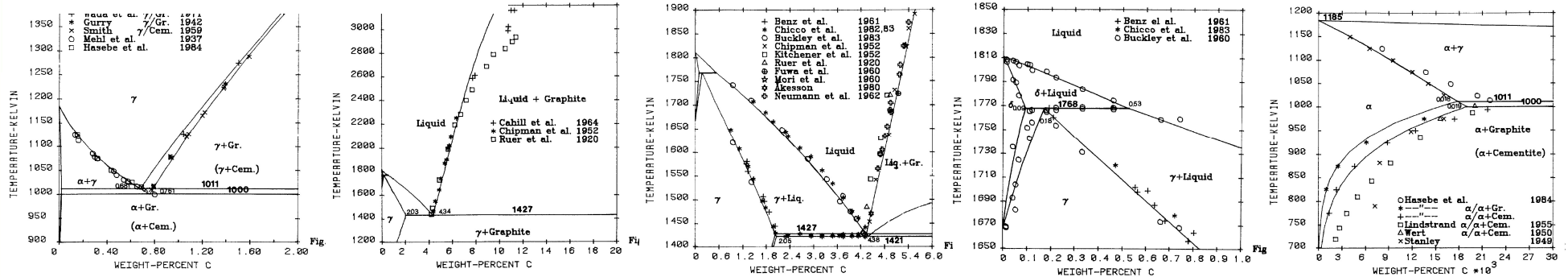
physical contribution  
(e.g. from magnetics)

Solution phase = solid solution (e.g. FCC, BCC, HCP....) or LIQUID.

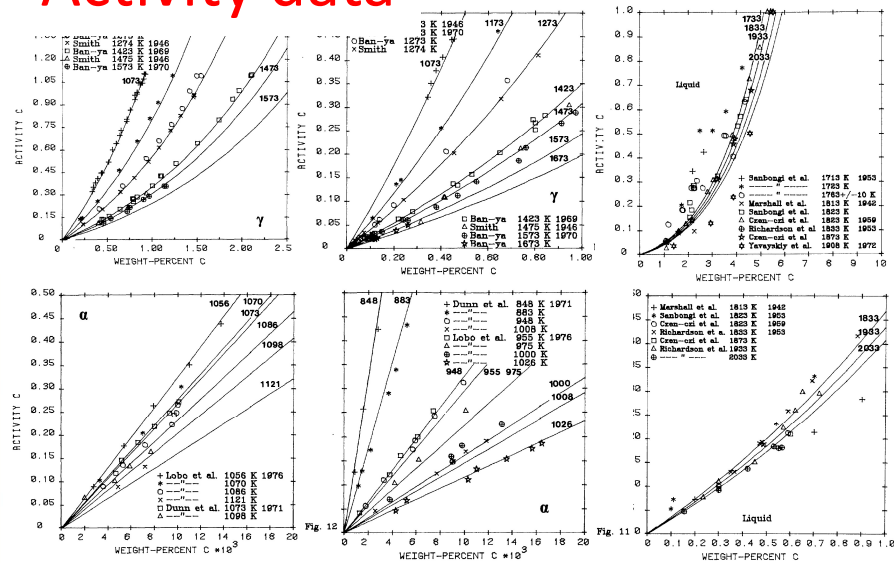
# Example Fe-C

Per Gustafson, 1985, *Scand. Journal of Metallurgy* 14(5):259-267

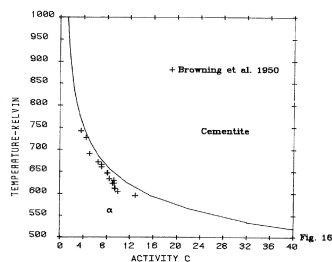
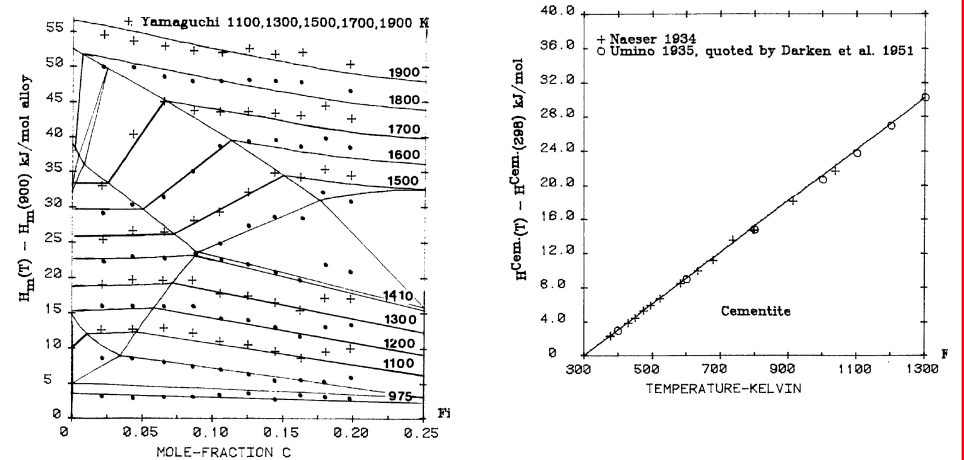
## Phase diagram data



## Activity data



## Enthalpy data



$$^0G_{Fe:C}^{hbcc} - ^0G_{Fe:Va}^{hbcc} - 3 G_C^{gra} = +322050 + 75.667 T$$

$$^0L_{Fe:Va,C}^{bcc} = -190 T$$

$$^0G_{Fe:C}^{fcc} - ^0G_{Fe:Va}^{fcc} - ^0G_C^{gra} = +77207 - 15.877 T$$

$$^0L_{Fe:Va,C}^{fcc} = -34671$$

$$^0G_{Fe:C}^{cem} - H_C^{SER} - 3 H_{Fe}^{SER} = -10745 + 706.04 T - 120.6 T \ln(T)$$

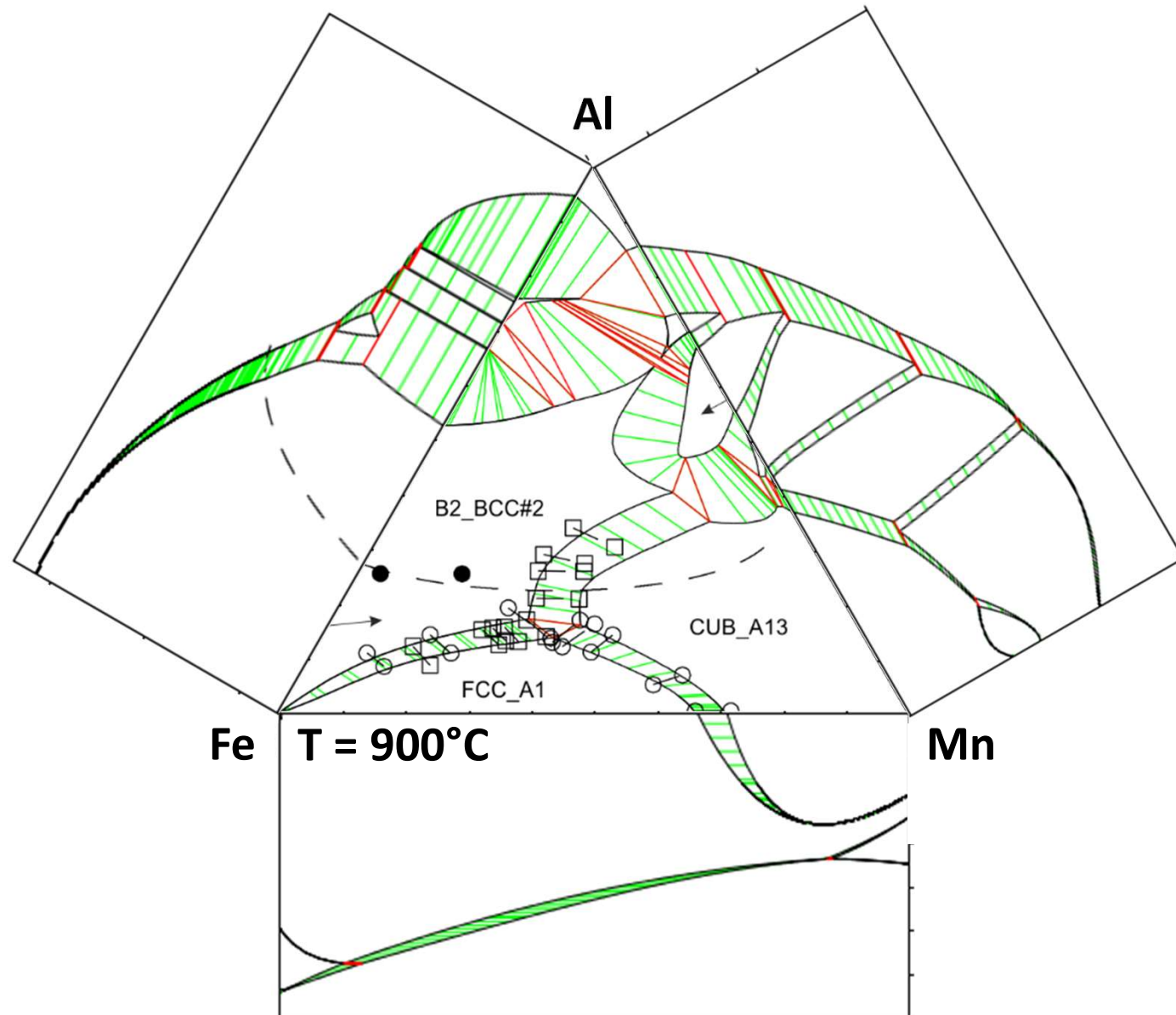
$$^0L_{Fe,C}^{liq} = -124320 + 28.5 T$$

$$^1L_{Fe,C}^{liq} = +19300$$

$$^2L_{Fe,C}^{liq} = +49260 - 19 T$$

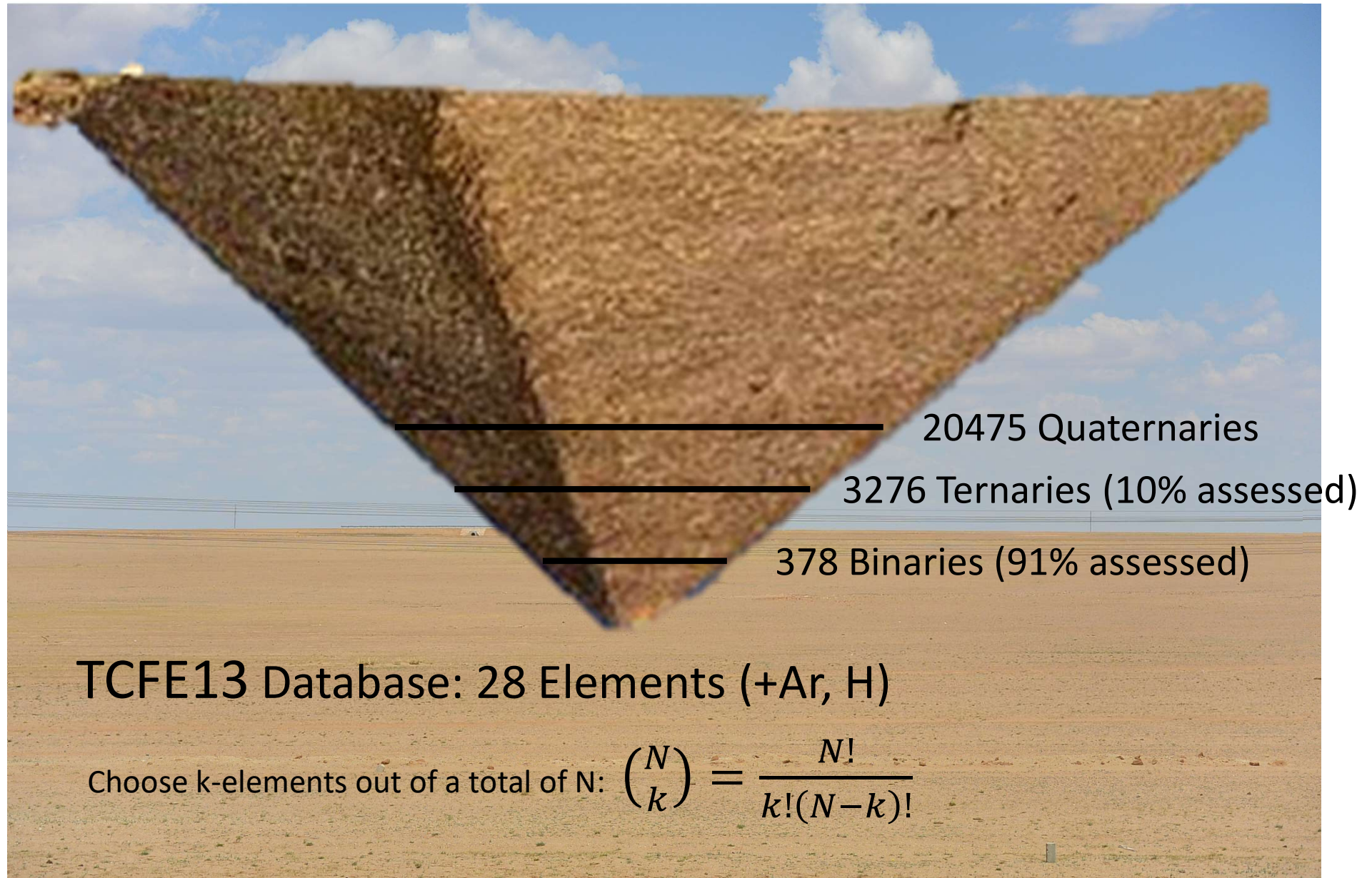
4 phases, >1000 experiments reproduced with 14 parameters

## From binaries to ternaries



# Extrapolation

→ How to predict multi-component materials?  
Extrapolation from binaries to ternaries, etc...



Carbides and nitrides are usually modelled with one sub-lattice for the metallic atoms and one for atoms that occupy the spaces in-between (interstitial positions), such as carbon or nitrogen. These interstitial sites are defined as a separate sub-lattice.

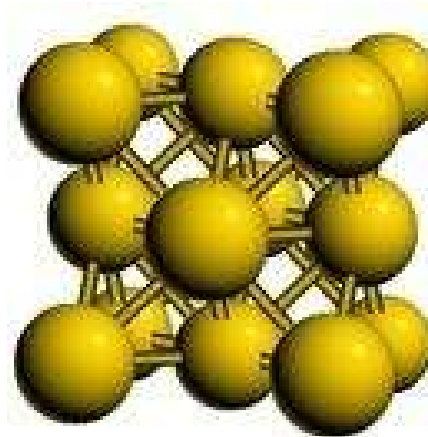
In many cases there are more than one sub-lattice for the metals.

The FCC carbonitride, e.g. TiC or VN is modelled as an a normal solid solution FCC phase, but in this case most of the interstitial sites are filled with carbon or nitrogen. This is handled in Thermo-Calc as second composition set of FCC and designated for instance FCC\_A1#2.

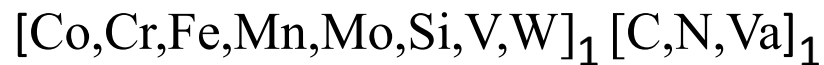
The HCP carbonitride,  $M_2C$  or  $M_2N$  is in the same way modelled as a second composition set of the HCP phase.

Other intermetallic phases can be modelled in many different ways.

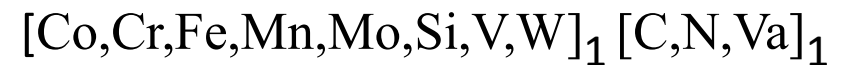
Fcc



**Austenite**



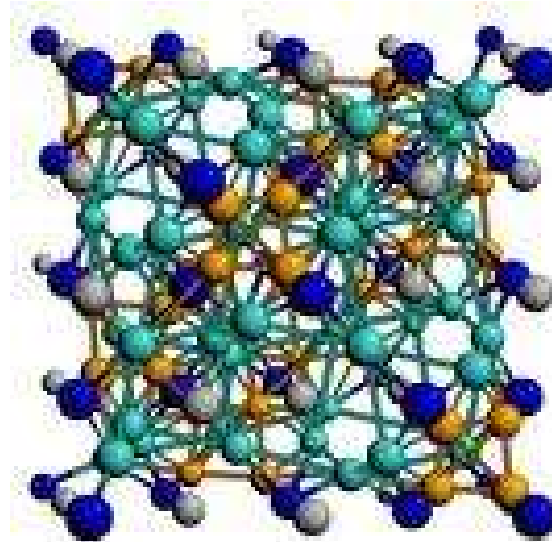
**Carbide/Carbonitride**



$$G_m^\phi = \sum_M \sum_I y_M y_I {}^\circ G_{M:I}^\phi + RT(a \sum_M y_M \ln y_M + c \sum_I y_I \ln y_I) + {}^E G_m^\phi + G_m^{\phi mg}$$

- ${}^\circ G_{M:I}$  is the Gibbs energy of formation of the compound  $\text{M}_a\text{I}_c$ .
- $y$  is the site fraction, and  $a$  and  $c$  are the site ratios.
- The excess and physical contributions are as for a regular solution on each sublattice.

## More complex structures needs more sublattices



### $M_6C$ Carbide

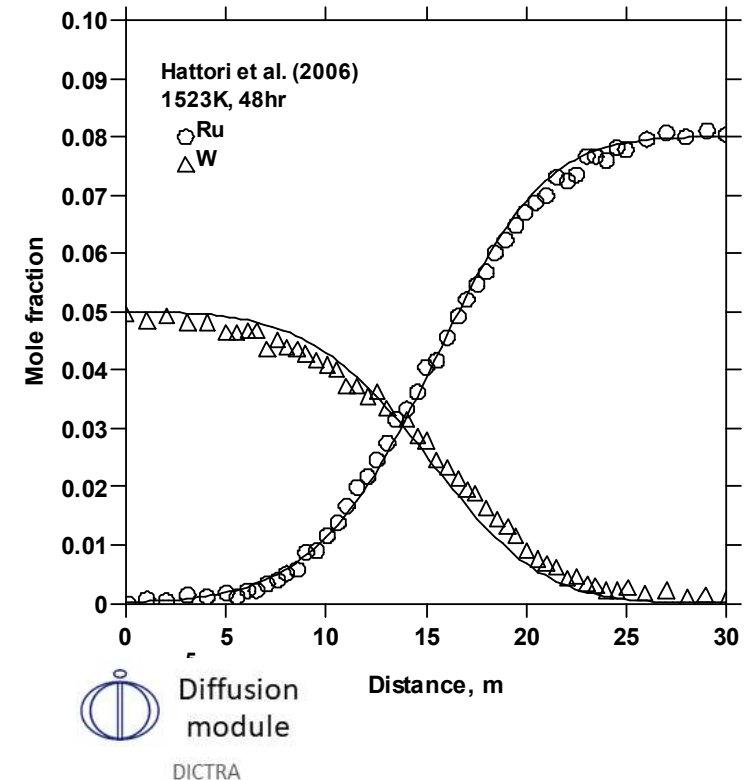
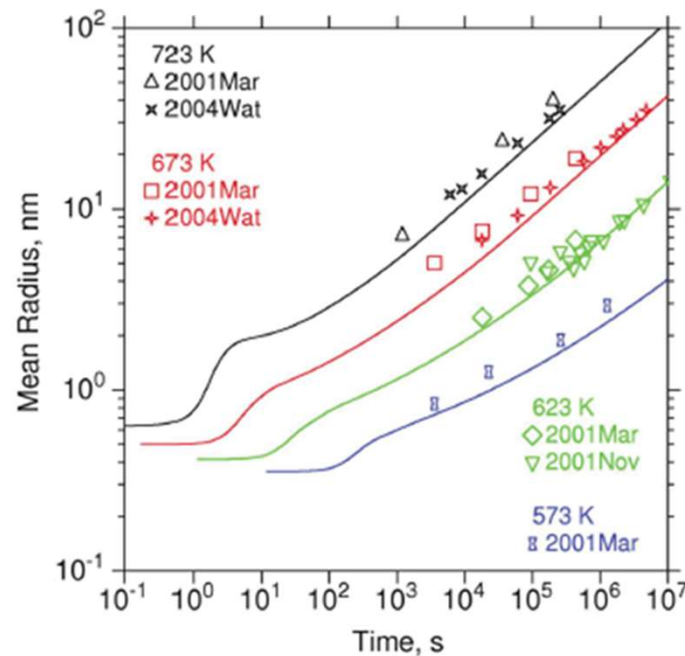


$$G_m = \sum y_I^1 y_J^2 y_K^3 {}^oG_{I:J:K:C} + RT \sum \sum n^S y_J^S \ln(y_J^S) + {}^E G_m$$

# Extensions of CALPHAD

CALPHAD was initially only applied for representing **thermochemical** and **phase-equilibrium** information (the first materials genome), but has since a long time been proven to be extended to other phase-based properties, e.g.

- ✓ Thermodynamic data
- ✓ Multicomponent mobility data
- ✓ Molar volume
- + Interfacial energy
- **Precipitation and growth**



# Later extensions of CALPHAD

- ✓ Thermodynamic data
- ✓ Multicomponent mobility data
- ✓ Molar volume
- + Interfacial energy
- ✓ Precipitation and growth

And more recently (from 2020 in our software) also:

- ✓ *Thermal conductivity*
- ✓ *Thermal resistivity*
- ✓ *Electrical conductivity*
- ✓ *Electrical resistivity*
- ✓ *Viscosity in Liquid phase*
- ✓ *Surface tension of Liquid phase*
- ✓ *Elastic moduli and elastic constants* (new - only in TCFE14 and TCTI6 so far)

## Three most common types of databases:

### **Substance database** (e.g. SSUB7, NUMT2):

Database for condensed phase compounds and gases

Advantage: Many elements, many compounds

Limitation: Not suitable for phase diagrams, phase transformations

### **Solution database** (e.g. TCFE14, TCNI13, SSOL9, TCOX14, etc):

Databases for alloys and solid solutions

Advantage: Describes phase diagrams, phase transformations

Limitation: Generally fewer elements than substance database/ SSOL6 has many elements but most assessments limited to binaries

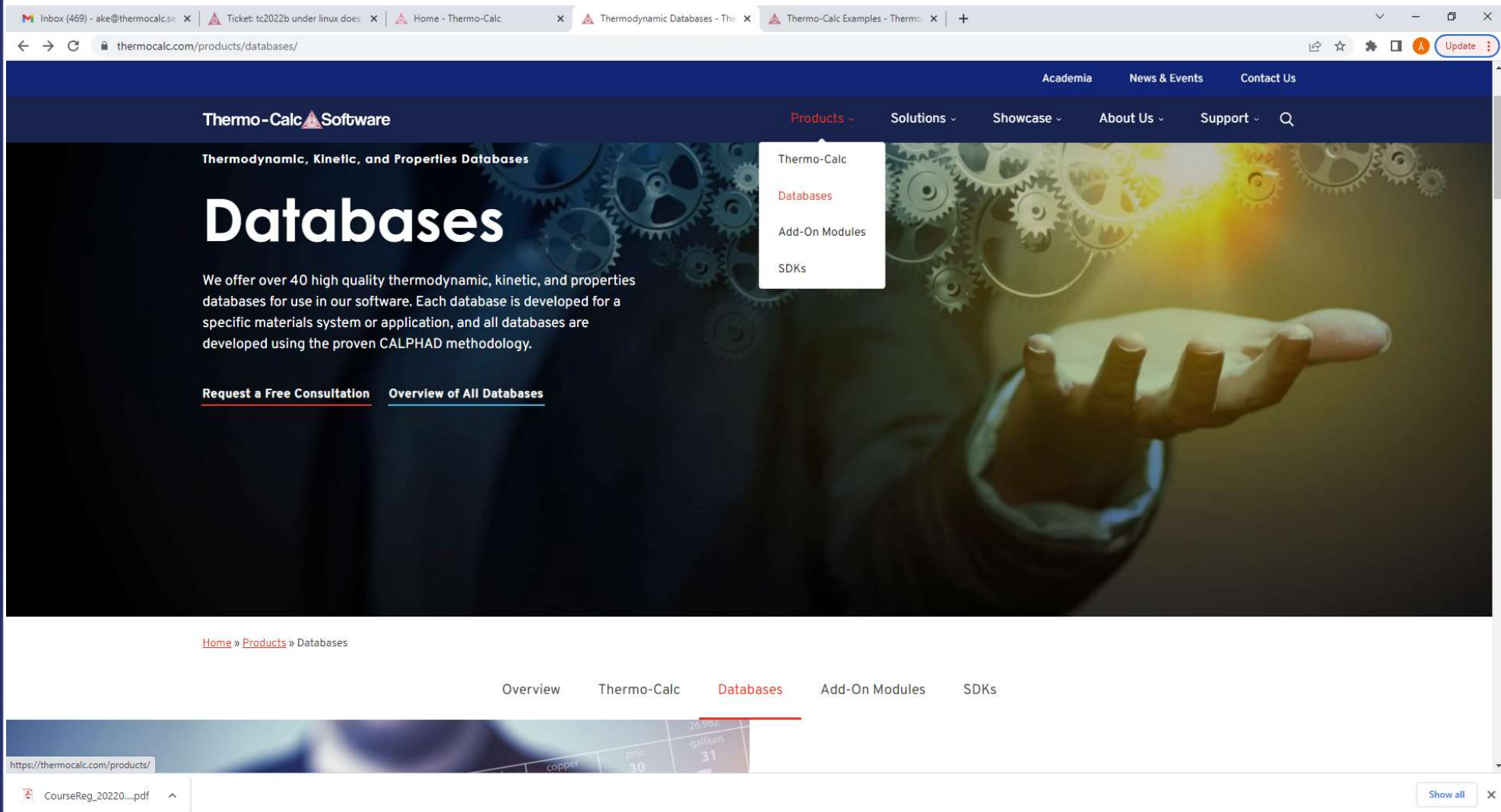
### **Aqueous databases** (e.g. TCAQ3, AQS2):

Advantage: Consists of various free cations and anions, inorganic and organic complexes

Limitation: Needs to be used in conjunction with substance or solution databases

# Selecting the right database(s) (2)

For a list of available thermodynamic and mobility databases refer to the database overview or [www.thermocalc.com](http://www.thermocalc.com)



The screenshot shows the Thermo-Calc Software website's 'Databases' page. The browser's address bar displays 'thermocalc.com/products/databases/'. The page features a dark blue header with navigation links: 'Academia', 'News & Events', 'Contact Us', 'Products', 'Solutions', 'Showcase', 'About Us', and 'Support'. A dropdown menu for 'Products' is open, showing 'Thermo-Calc', 'Databases' (highlighted), 'Add-On Modules', and 'SDKs'. The main content area has a background image of a hand holding a glowing orb with gears. The text reads: 'Thermodynamic, Kinetic, and Properties Databases', 'Databases', and 'We offer over 40 high quality thermodynamic, kinetic, and properties databases for use in our software. Each database is developed for a specific materials system or application, and all databases are developed using the proven CALPHAD methodology.' Below this are links for 'Request a Free Consultation' and 'Overview of All Databases'. A breadcrumb trail at the bottom reads 'Home » Products » Databases'. A secondary navigation bar includes 'Overview', 'Thermo-Calc', 'Databases' (highlighted), 'Add-On Modules', and 'SDKs'. At the bottom, a partial periodic table is visible, showing elements like copper, zinc, and gallium. A 'Show all' button is located in the bottom right corner.

Thermo-Calc Software

Thermodynamic, Kinetic, and Properties Databases

# Databases

We offer over 40 high quality thermodynamic, kinetic, and properties databases for use in our software. Each database is developed for a specific materials system or application, and all databases are developed using the proven CALPHAD methodology.

[Request a Free Consultation](#) [Overview of All Databases](#)

[Home](#) » [Products](#) » Databases

[Overview](#) [Thermo-Calc](#) [Databases](#) [Add-On Modules](#) [SDKs](#)

[Show all](#)

# Selecting the right database(s) (2)

For a list of available thermodynamic and mobility databases refer to the database overview or [www.thermocalc.com/products/databases](http://www.thermocalc.com/products/databases)



## Databases

The quality of the predictions in Thermo-Calc is strongly dependent on the quality of the databases because they provide the data for the calculations. This makes the databases as important, if not more so, than the software itself.

Thermo-Calc Software has long experience in the field of database generation using the proven CALPHAD methodology. We employ a highly qualified team of people working on database development internally and through international collaboration projects. With our kinetic, properties, and thermodynamics databases, you can rest assured that you are working with the most advanced CALPHAD databases available.

[Learn about the CALPHAD methodology](#)

## Our Thermodynamic, Kinetic, and Properties Databases

|                                                              |                                                                                      |                                                                                      |
|--------------------------------------------------------------|--------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
| <b>Steel and Fe-Alloys</b><br><a href="#">Read more</a>      | <b>Nickel-based Alloys</b><br><a href="#">Read more</a>                              | <b>Aluminium-based Alloys</b><br><a href="#">Read more</a>                           |
| <b>Magnesium-based Alloys</b><br><a href="#">Read more</a>   | <b>Copper-based Alloys</b><br><a href="#">Read more</a>                              | <b>Titanium and Titanium<br/>Aluminide-based Alloys</b><br><a href="#">Read more</a> |
| <b>Noble Metal-based Alloys</b><br><a href="#">Read more</a> | <b>High Entropy Alloys</b><br><a href="#">Read more</a>                              | <b>Solder Alloys</b><br><a href="#">Read more</a>                                    |
| <b>Silicon-based Alloys</b><br><a href="#">Read more</a>     | <b>Metal Oxide Solutions</b><br><a href="#">Read more</a>                            | <b>Molten Salts</b><br><a href="#">Read more</a>                                     |
| <b>Cemented Carbides</b><br><a href="#">Read more</a>        | <b>Electronic Materials</b><br><a href="#">Read more</a>                             | <b>Aqueous Solutions</b><br><a href="#">Read more</a>                                |
| <b>Minerals</b><br><a href="#">Read more</a>                 | <b>General Alloys and Pure<br/>Substances from SGTE</b><br><a href="#">Read more</a> | <b>Nuclear Materials from IRSN</b><br><a href="#">Read more</a>                      |



**Thermo-Calc  
Software**

## TCHEA7 Assessed Binary Systems

[illegible]

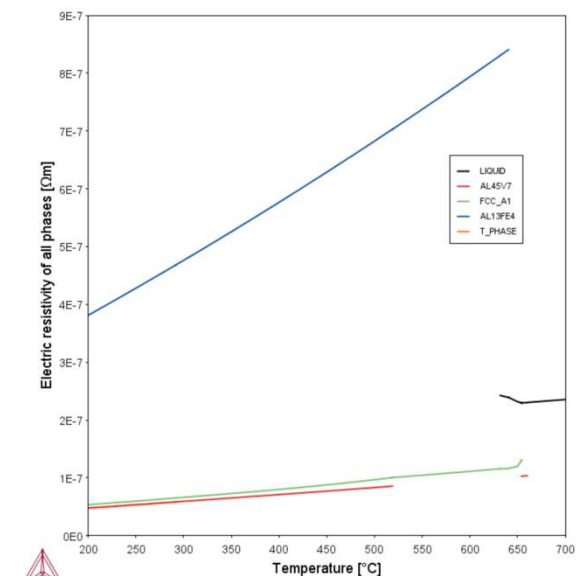
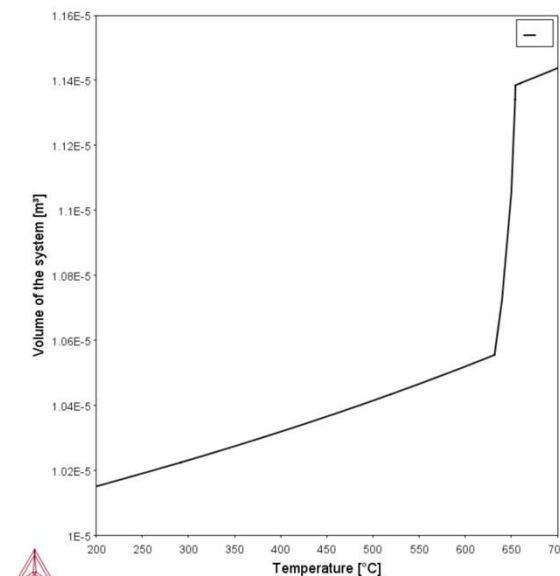
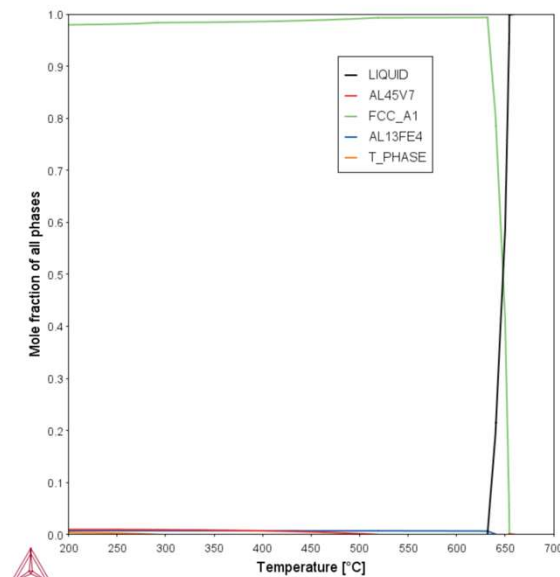
Step 3: Al alloy UNS A\_96053.  
Volume change at  
solidification and other  
properties.

# Property diagrams for Al-Alloy 6053

## Step example 3.

Calculate different properties as a function of T for this alloy:  
Al – 1.2 Mg – 0.35 Fe – 0.25 Cr – 0.1 Cu – 0.1 Zn (wt-%)

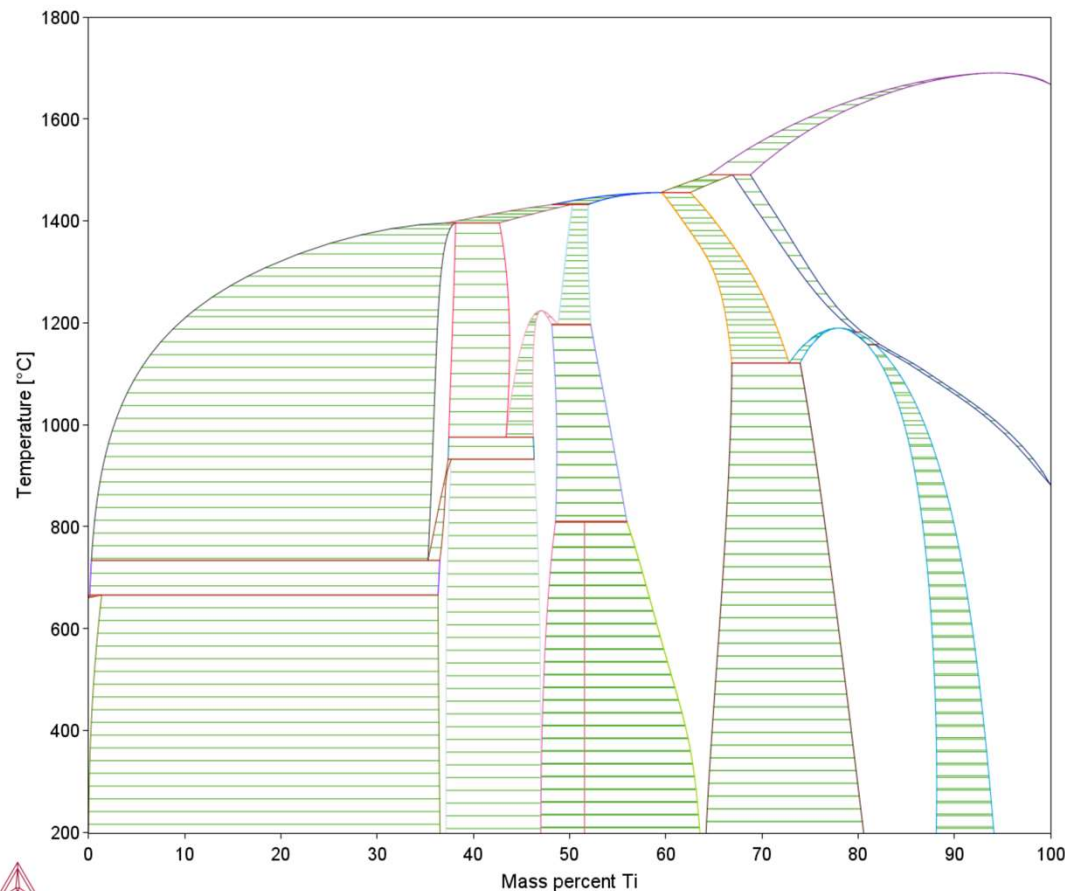
Use the “Load Material” option in System Definer. Remember to make sure the database is TCAL9.



Map calculations –  
two axes (or more)  
→ Phase diagrams

# Binary phase diagram

## Al-Ti Binary

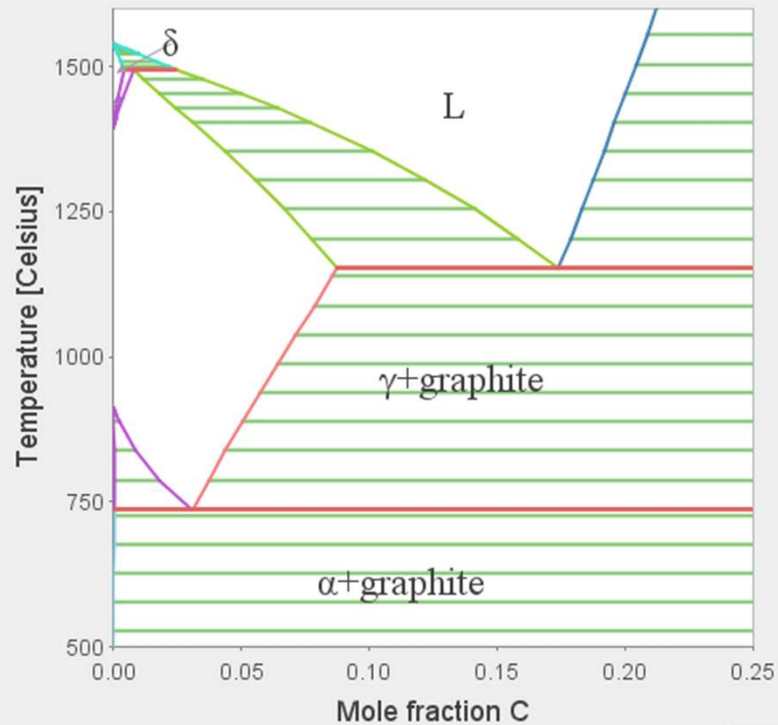


Use the "Binary Phase Diagram" template.

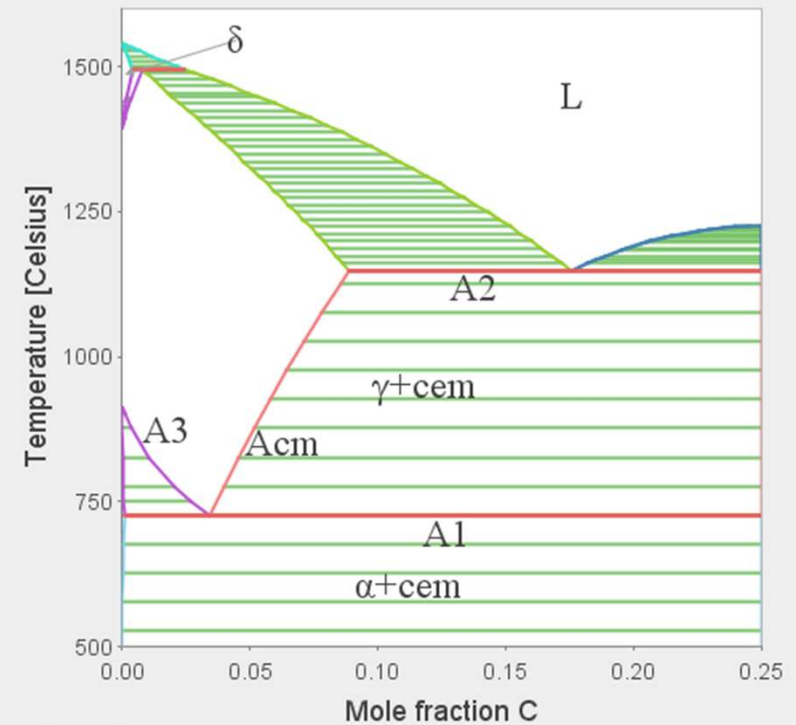
TCBIN, the special binary database, is default.

But also several other databases can be used.  
This diagram from TCAL8.

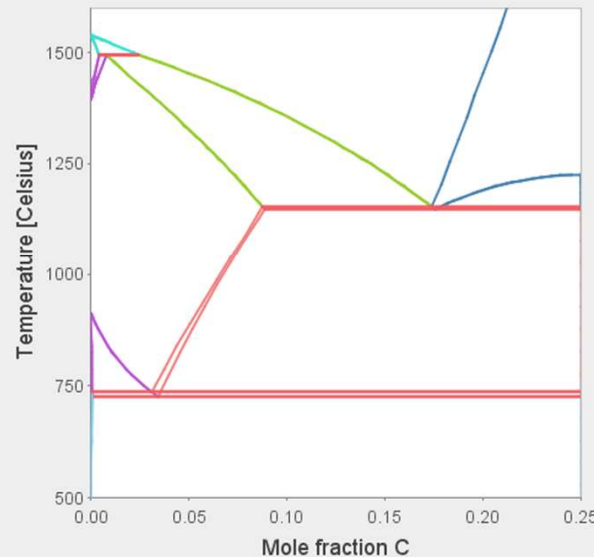
# Phase diagram calculations



Stable diagram



Metastable diagram



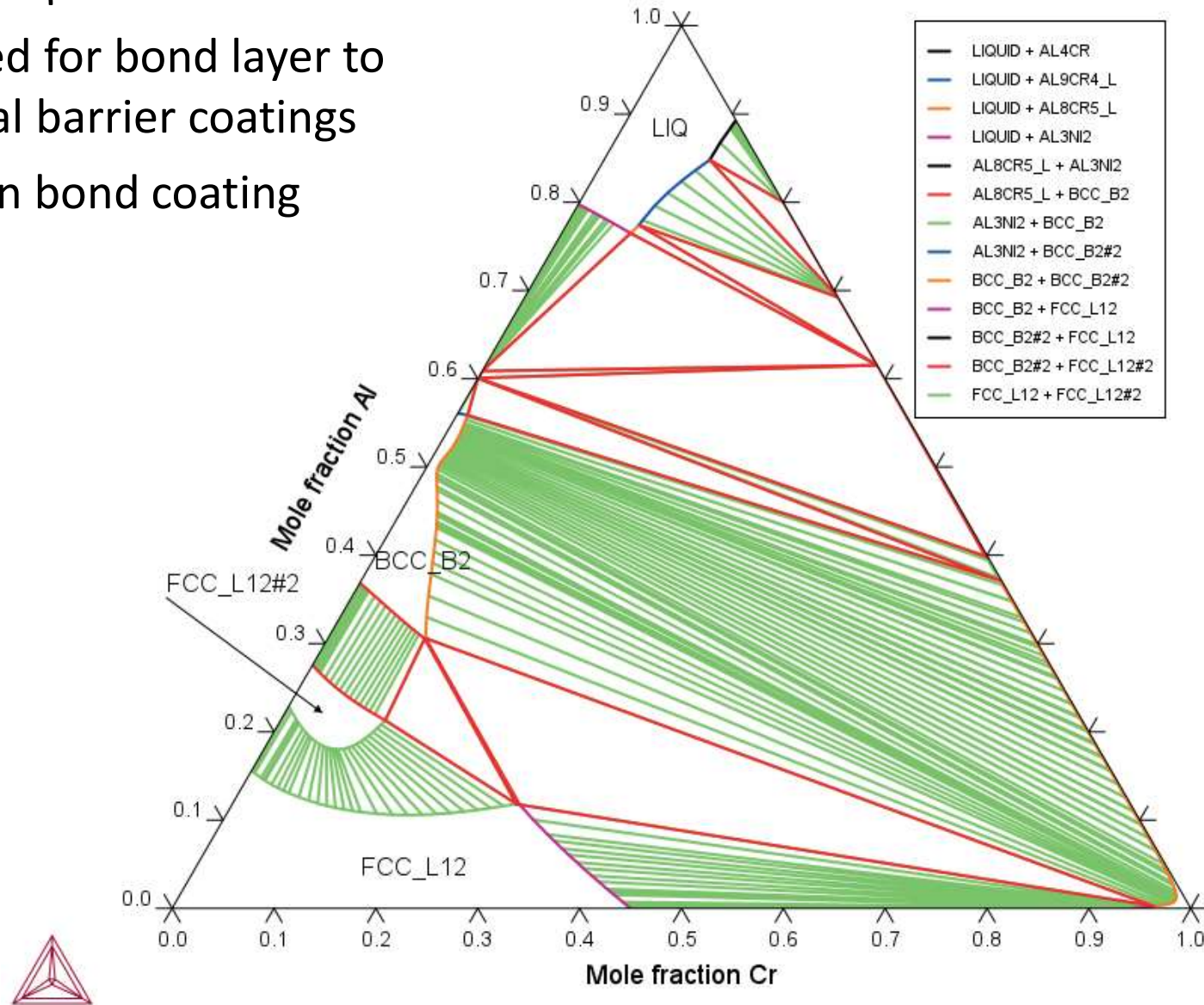
Combined diagram

# Ternary Isothermal Section

Ni-Al shows  $\gamma + \gamma'$

Ni-Cr-Al is used for bond layer to  
join to thermal barrier coatings

Used to design bond coating  
composition



Isothermal section of Ni-Cr-Al at 1000°C

# Multicomponent Phase Diagrams

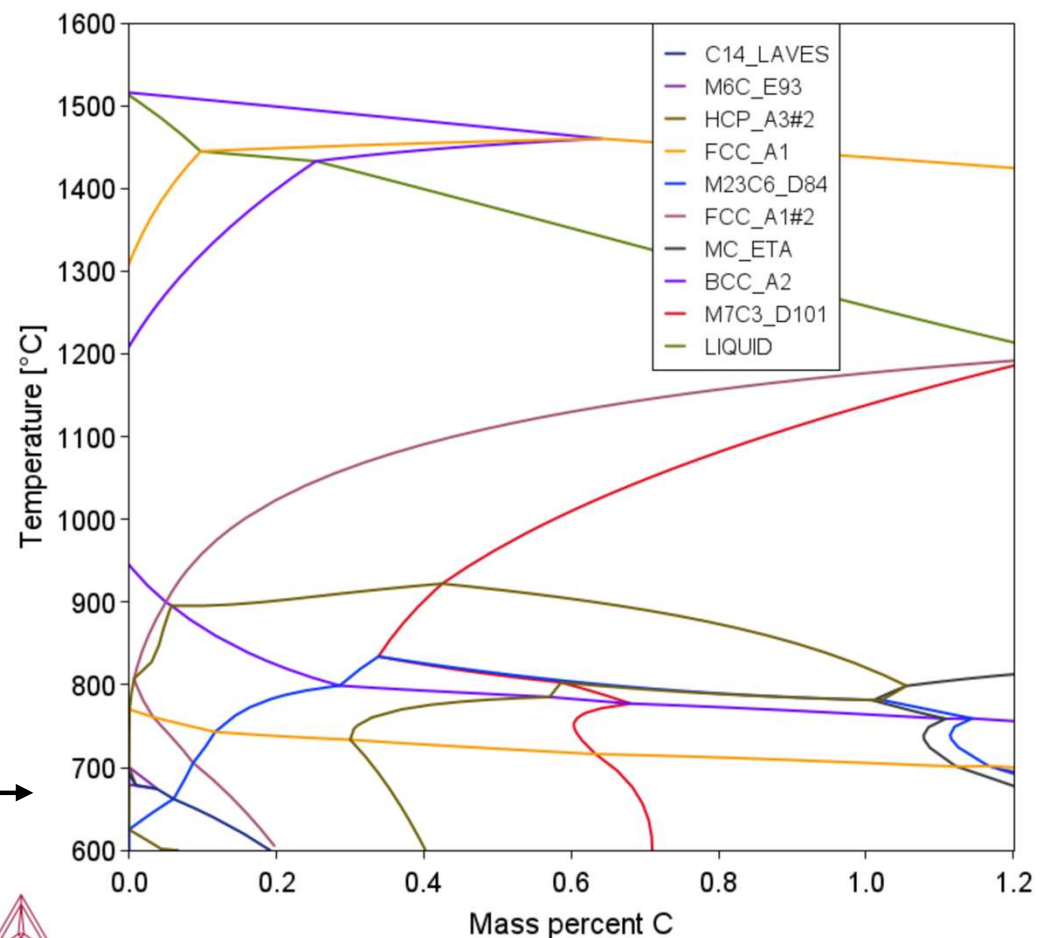
When making phase diagrams of more complicated alloys (more components) the diagrams can get very confusing

Because it's not a binary, the tie-lines do not lie in the plane of the calculation so the lever rule is not possible

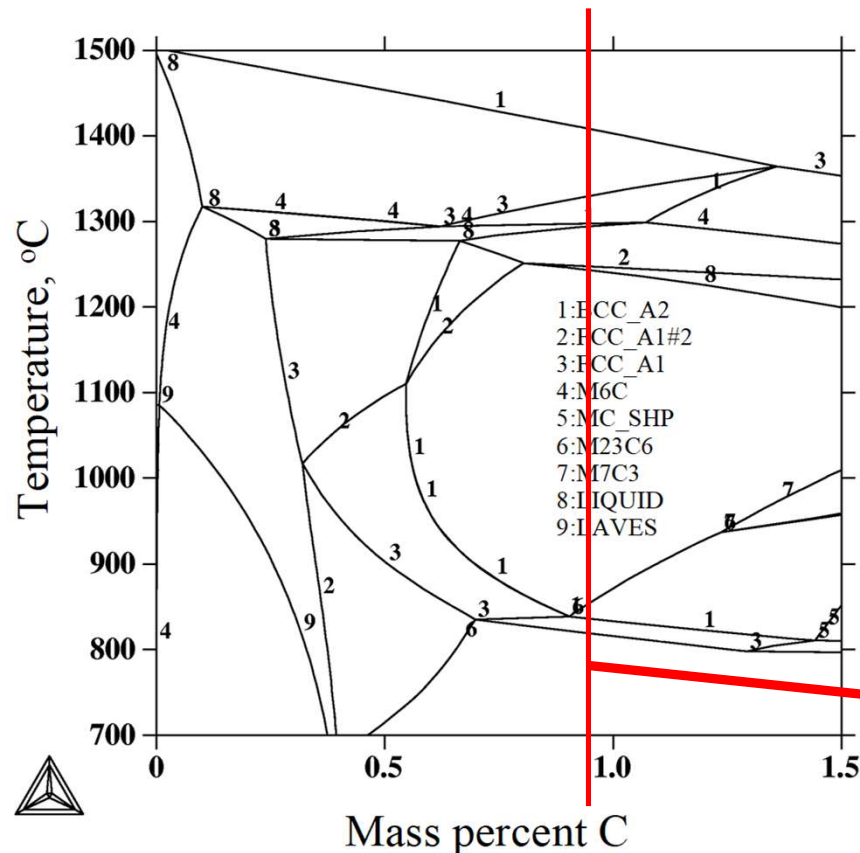
Hard to label the diagram as well with so many small regions

Coloured lines indicate a phase is stable on one side of the line and not stable on the other side

Tool steel with Fe-5 Cr-1.5 Mo-1.5 Ni-1 V-0.5 Mn – (0--1.2) C

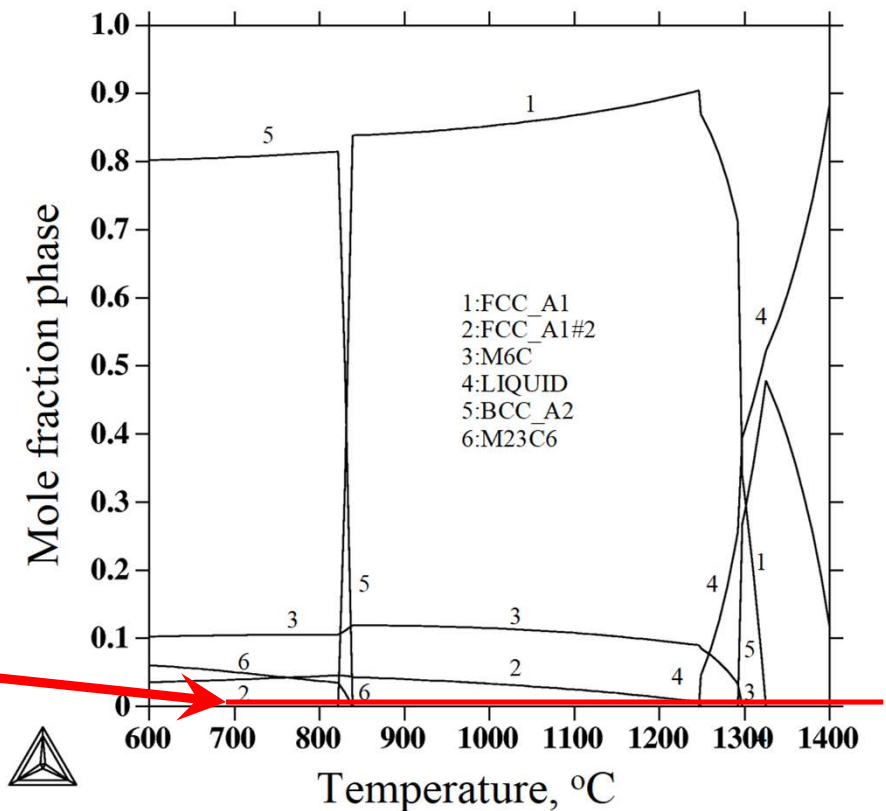


## Example: Carbon in M42 High Speed Steel



### Phase diagram for a M42 high speed steel.

The lines represent where a phase appears or disappears. The alloy is Fe-4Cr-5Mo-8W-2V-0.3Mn-0.3Si-C(wt%). **Isolethal section.**



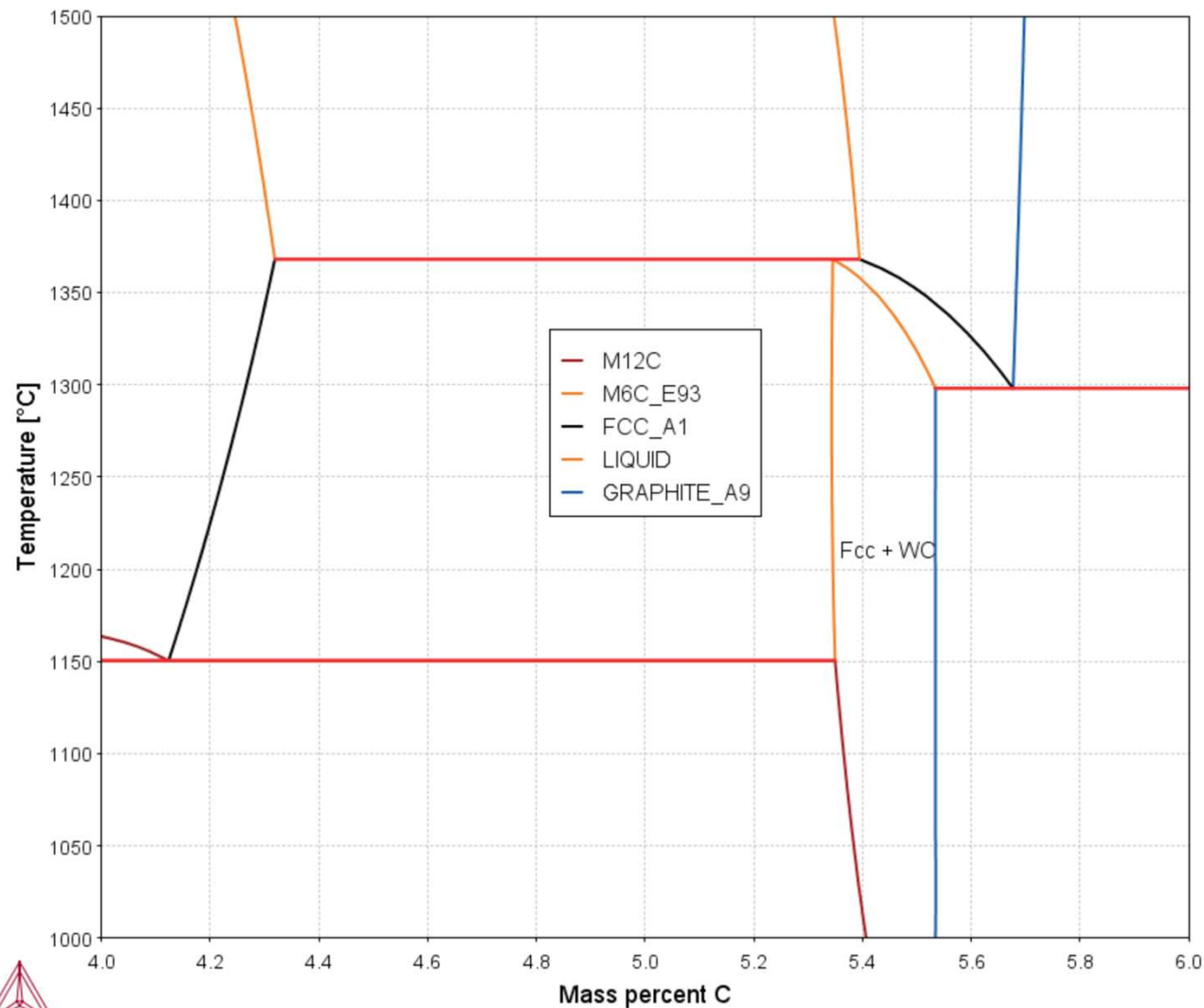
### Property diagram for a M42 high speed steel.

Shows how the fractions of the phases in the system vary with temperature. The alloy is Fe-4Cr- 5Mo-8W-2V-0.3Mn-0.3Si-0.9C.

# Map 1: Phase diagram for a cemented carbide.

# Cemented carbide phase diagram. Map ex. 1.

Typical hard metal (cemented carbide): W + C + 10 wt-% Co binder.  
Calculate this diagram. Then replace 3 wt-% Co with Fe and  
calculate a second diagram.



# Questions & Answers

Map 2: Phase diagram for a  
HEA with one element  
replacing all the other.

# High Entropy Alloys

## (= Multi Principal-Element Alloys)

**High-entropy alloys (HEAs)** are alloys that are formed by mixing equal of relatively large proportions of (usually) five or more elements.

The entropy increase of mixing is substantially higher when there is a larger number of elements in the mix, and their proportions are nearly equal.

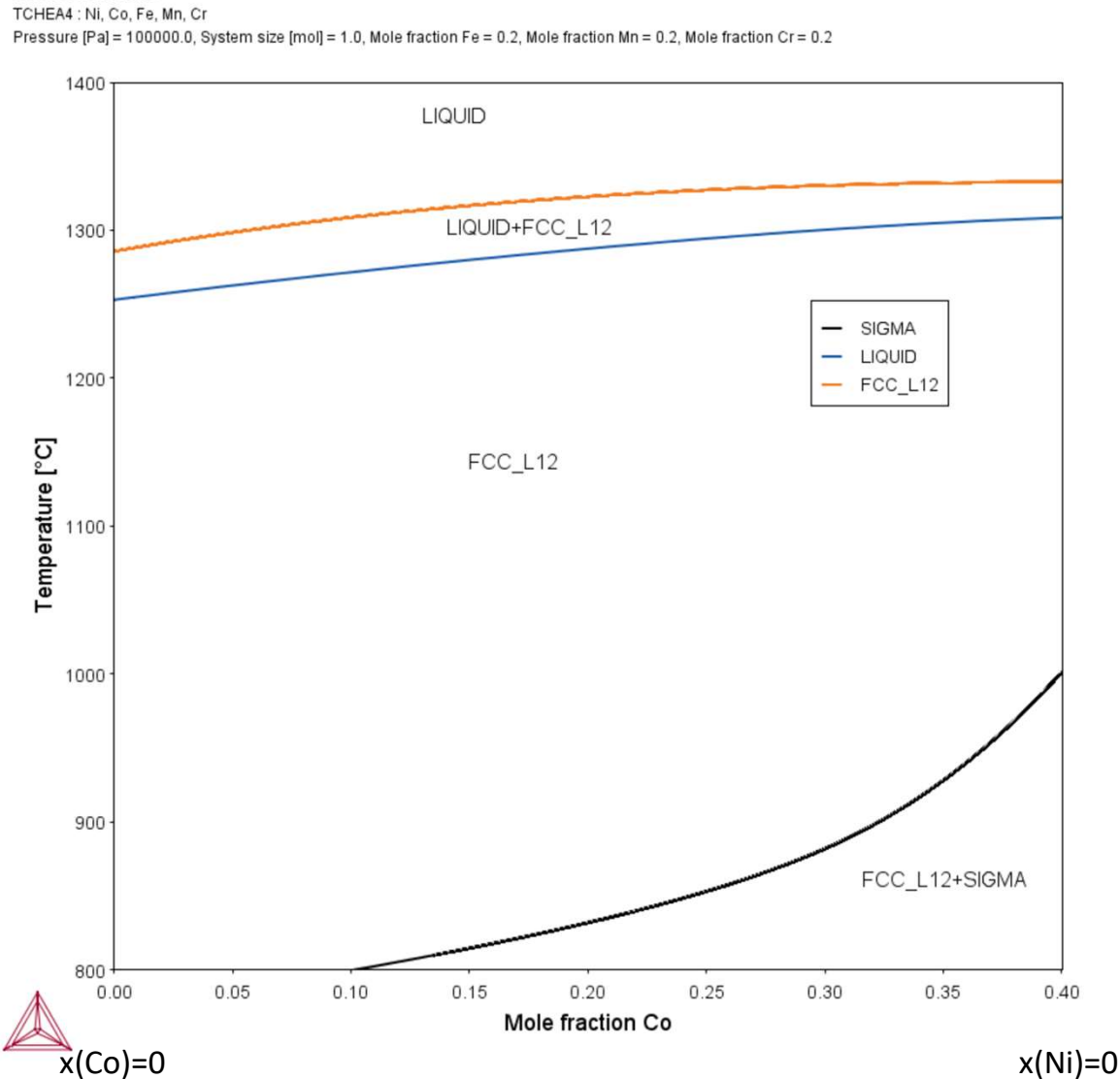
There is no universally agreed-upon definition of a **HEA**. The original definition of **HEAs** was alloys containing at least 5 elements with concentrations between 5 and 35 atomic percent. Later research has suggested that this definition could be expanded.

An alternative name for **HEAs** is **Multi-Principal Element Alloys**.

From Wikipedia, the free encyclopedia.

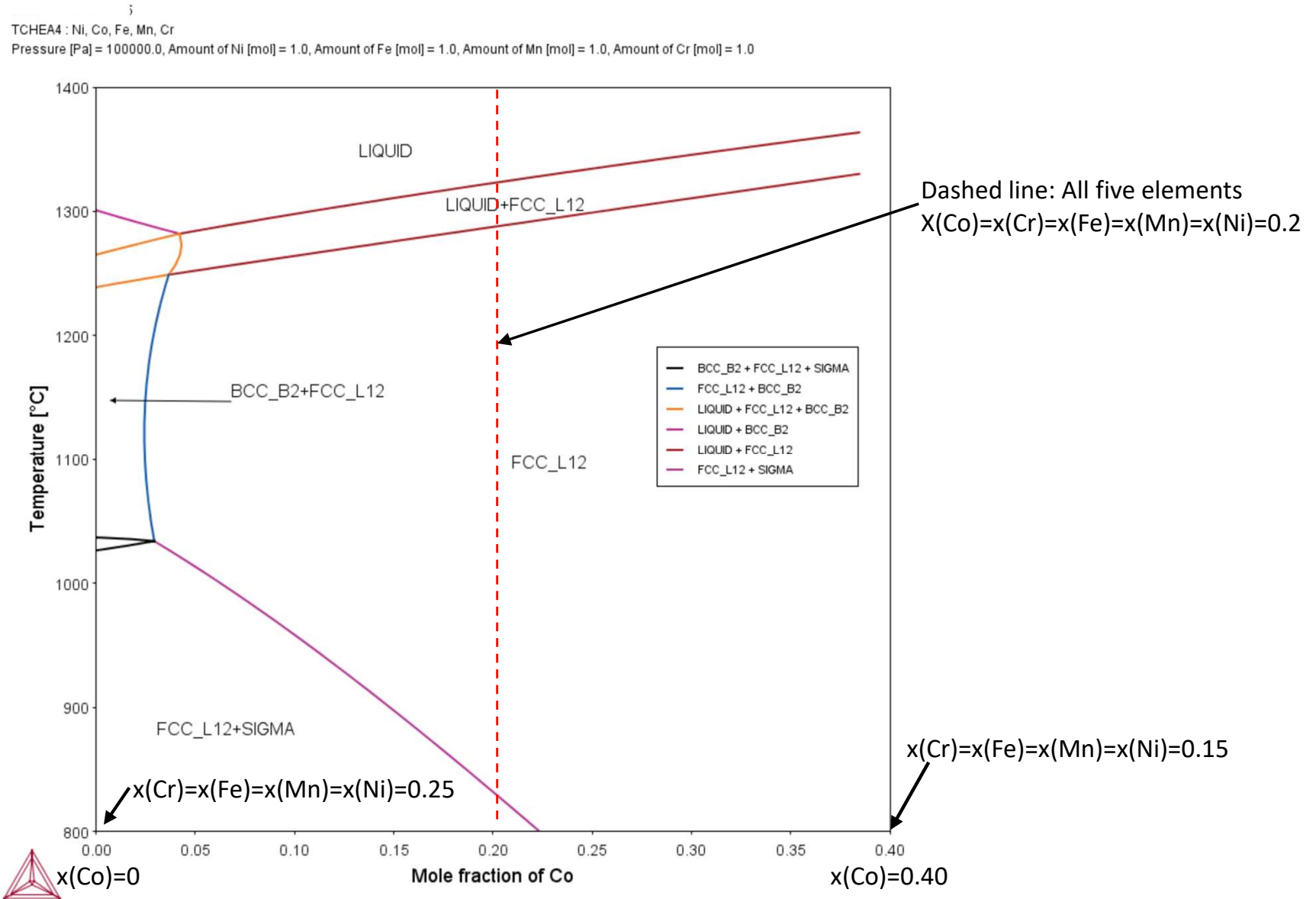
# High Entropy Alloy phase diagram, Map ex. 2

This is a standard phase diagram with Co replacing Ni with conditions  $x(\text{Fe}) = x(\text{Mn}) = x(\text{Cr}) = 0.2$ . This means  $x(\text{Ni}) + x(\text{Co}) = 0.4$



# High Entropy Alloy phase diagram, Map ex. 2

Adding Co to an alloy with equal parts Cr – Fe – Mn – Ni (in mole-fraction).  
Co is not replacing just one base metal (unlike standard phase diagrams).



# Map 3: Base metal to Weld phase diagram.

## Multicomponent "mapped" diagrams, Map ex. 3



Calculate a phase diagram between two high alloyed stainless steels. All alloying elements are changing along the x-axis. This used to require functions as conditions.

(Functions can be written in console mode syntax. Must use  $W(ii)$  = Weight-fraction and not wt-%.)

**Material to Material Calculator** is a relatively new feature. This template makes such a calculation much easier to set up.

**Base**    Fe – 0.0 Ni – 20 Cr – 0.2 C (wt-%)

**Filler**    Fe – 20 Ni – 25 Cr – 0.15 C (wt-%)

See next slide.

# Multicomponent "mapped" diagrams, Map ex. 3

Configuration

Material to Material Calculator 1

Conditions Functions Options

Composition unit: Mass percent

Condition Definitions

Temperature: Celsius 1500

Pressure: Pascal 100000.0

Fraction of second material: 0.99

Dependent component: Fe

Activity conditions: ☐

First material

Material name: Base

Composition Cr: 20

Composition Ni: 0

Composition C: 0.2

Load material

Save material as...

Second material

Material name: Filler

Composition Cr: 25

Composition Ni: 20

Composition C: 0.15

Load material

Save material as...

Calculation Type

☐ Single equilibrium ☐ One axis ☒ Phase diagram

Axis Definitions

| Quantity                | Min | Max  | Step division | Type               |
|-------------------------|-----|------|---------------|--------------------|
| Mass fraction of Filler | 0.0 | 1.0  | 50.0          | Linear - min no. c |
| Temperature             | 600 | 1600 | 50.0          | Linear - min no. c |

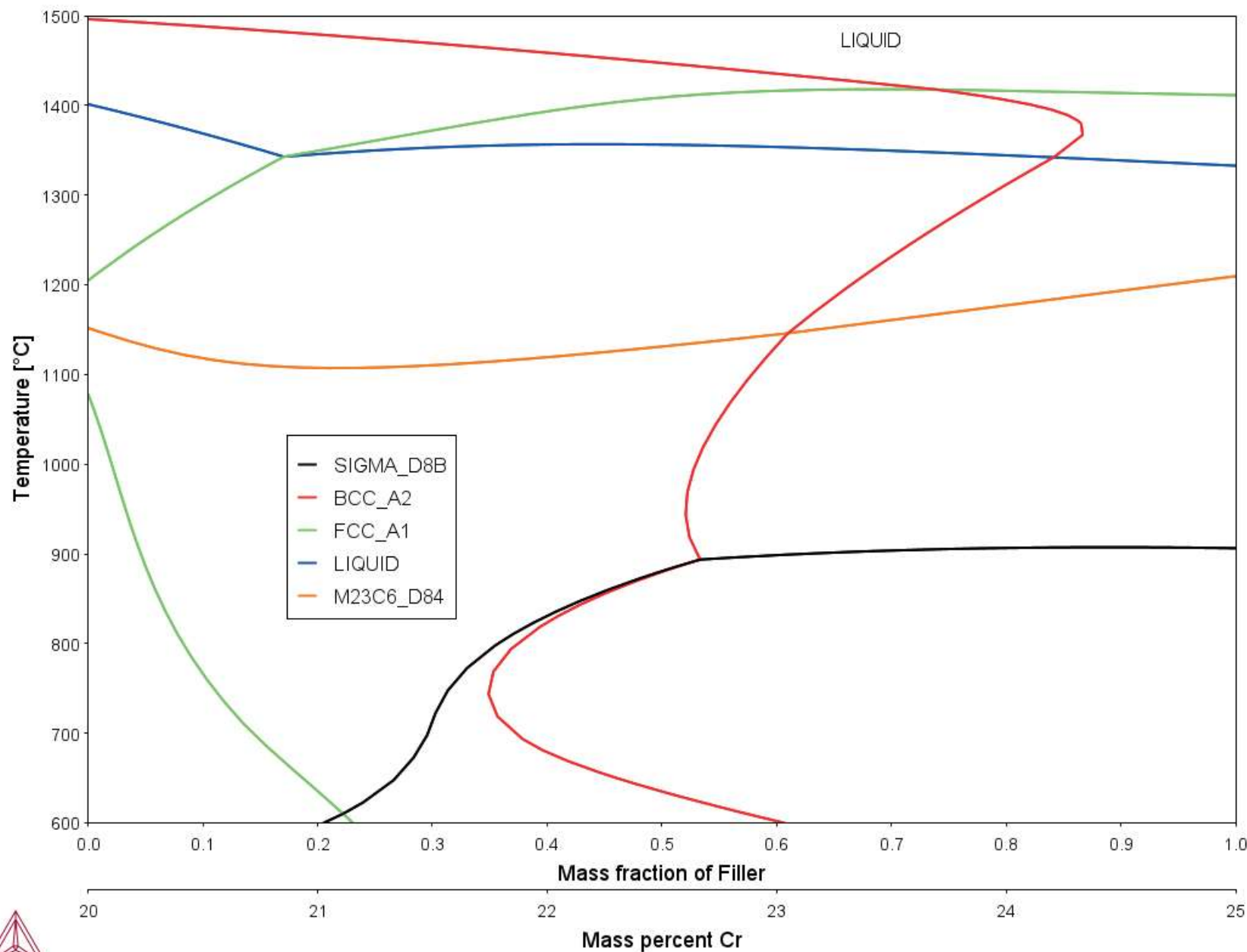
3 types of calculations,  
Phase diagram is one.

# Multicomponent "mapped" diagrams, Map ex. 3

2022.03.15.15.43.48

TCFE12 : Fe, Cr, Ni, C

Mass percent Cr = 20.0, Mass percent Ni = 0.0, Mass percent C = 0.2



# Questions & Answers

# Home Assignment 2

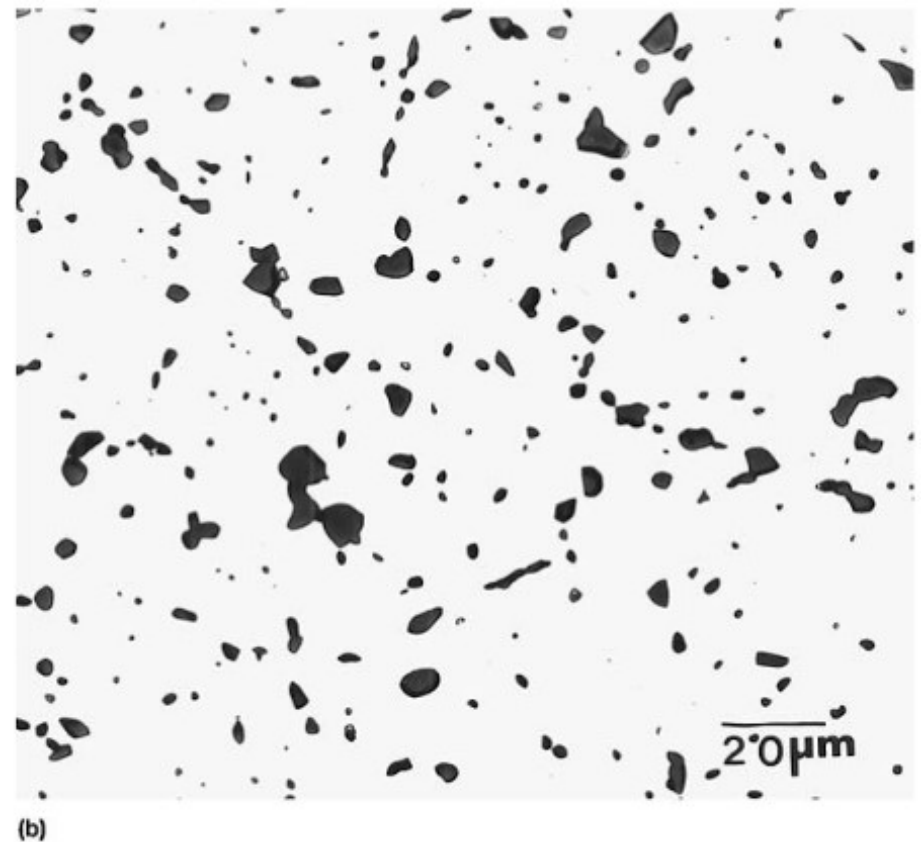
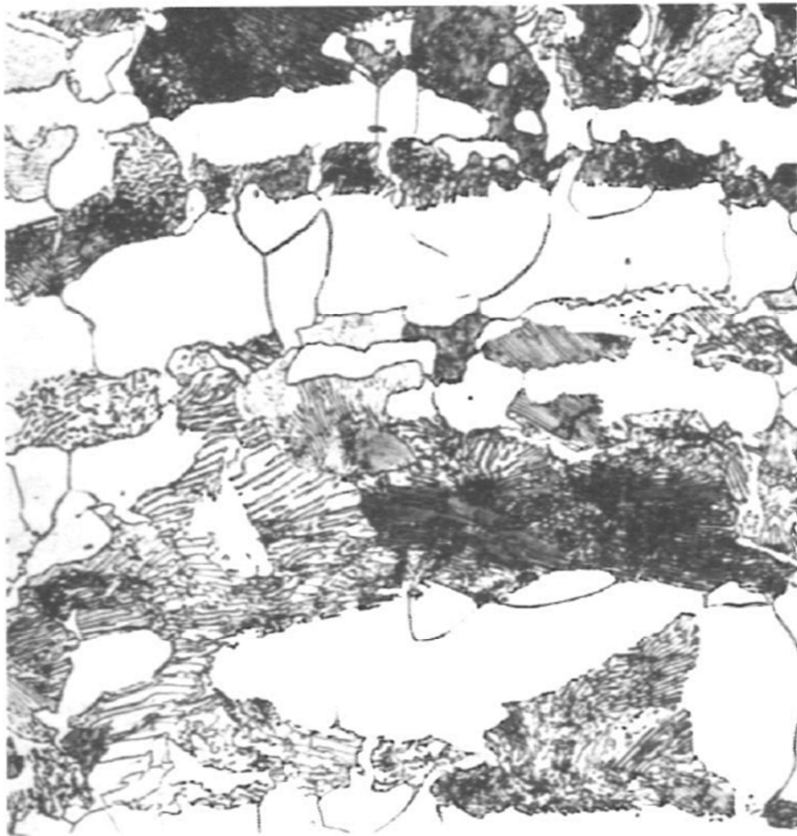
## Home Assignment 2

Calculate Equilibrium at 600 °C for the following steel:

- AISI 1040 with Fe (bal.) – 0.4C - 0.7Mn (wt-%)

Which microstructure aligns with your result?

Is this Graphite or  $\text{Fe}_3\text{C}$  (Cementite)?



From ASM International: Heat Treaters Guide (1995).

# Extra if there is time:

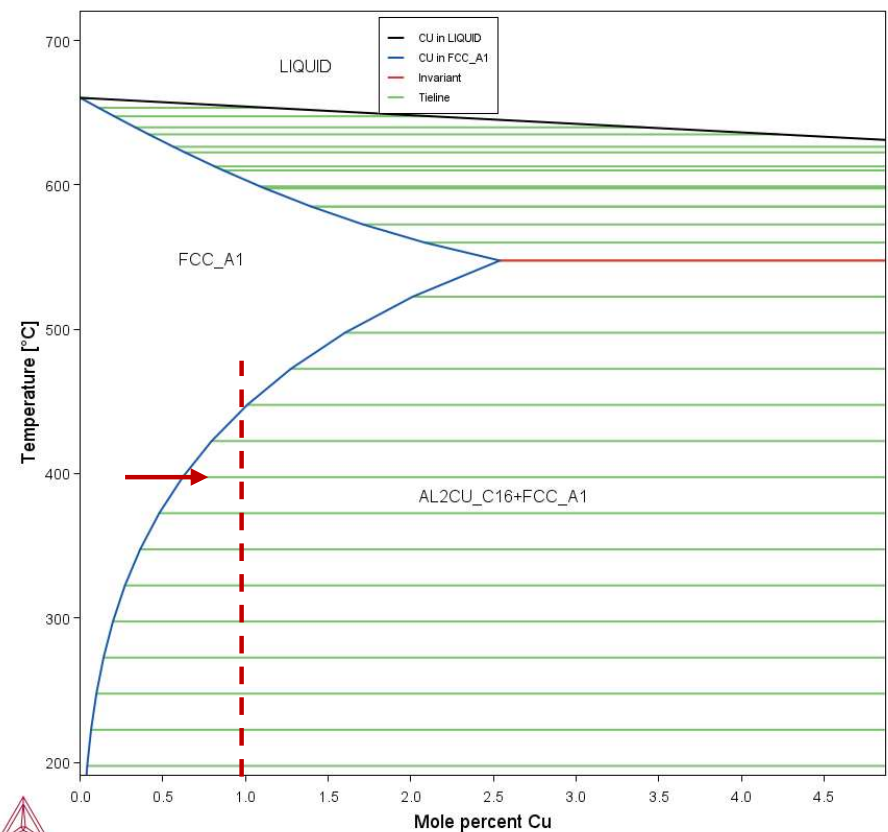
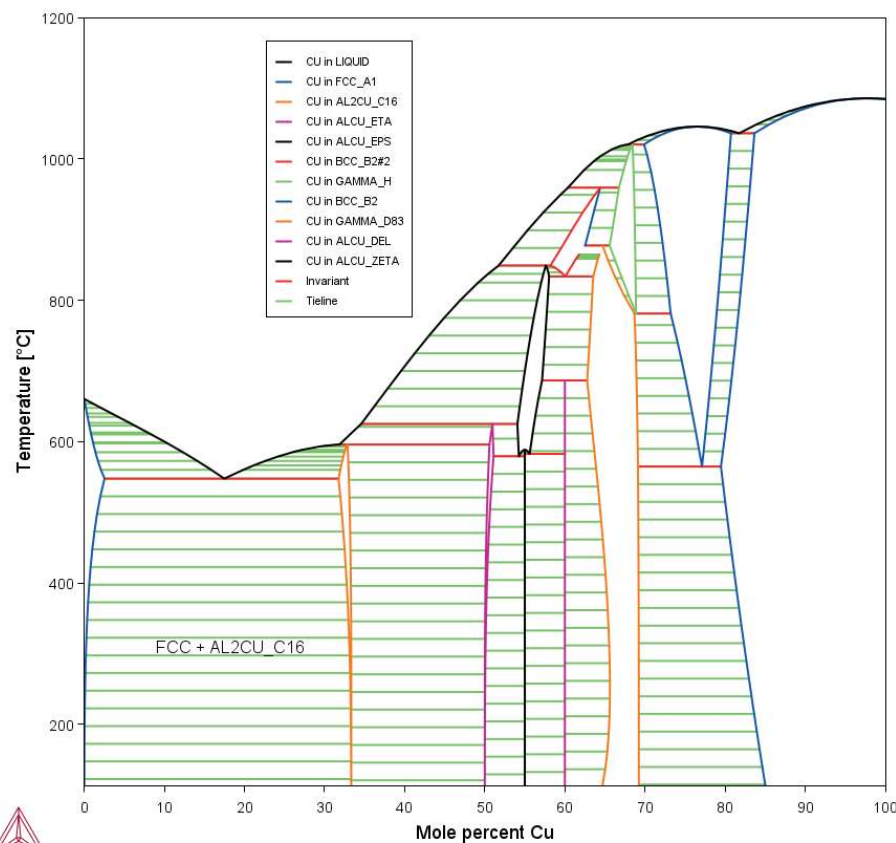
Example on driving force  
(dormant phase status)

# Stable and metastable phases in Al-Cu

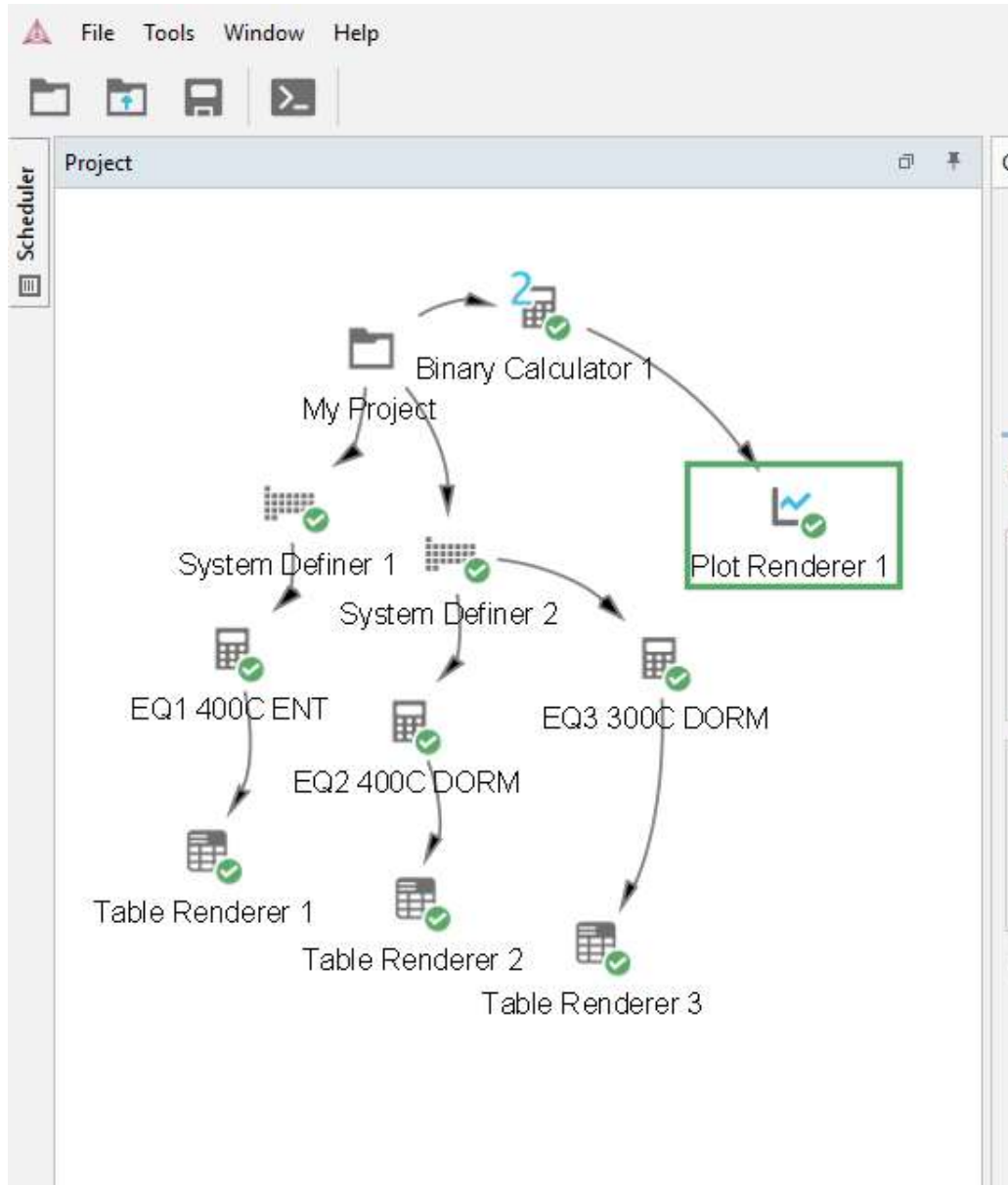
Using the same binary system from yesterday, Al-Cu with 1 mol-% Cu

What does different values of “normalized driving force” mean?

This is a dimensionless variable, in console syntax DGM(phase).



# Stable and metastable phases in Al-Cu



1. Select TCAL9 and Al, Cu
2. De-select all phases
3. Select fcc, AL2CU, Theta\_prime and Theta\_dprime
4. Calculate at 400 C, 1 mol-% Cu

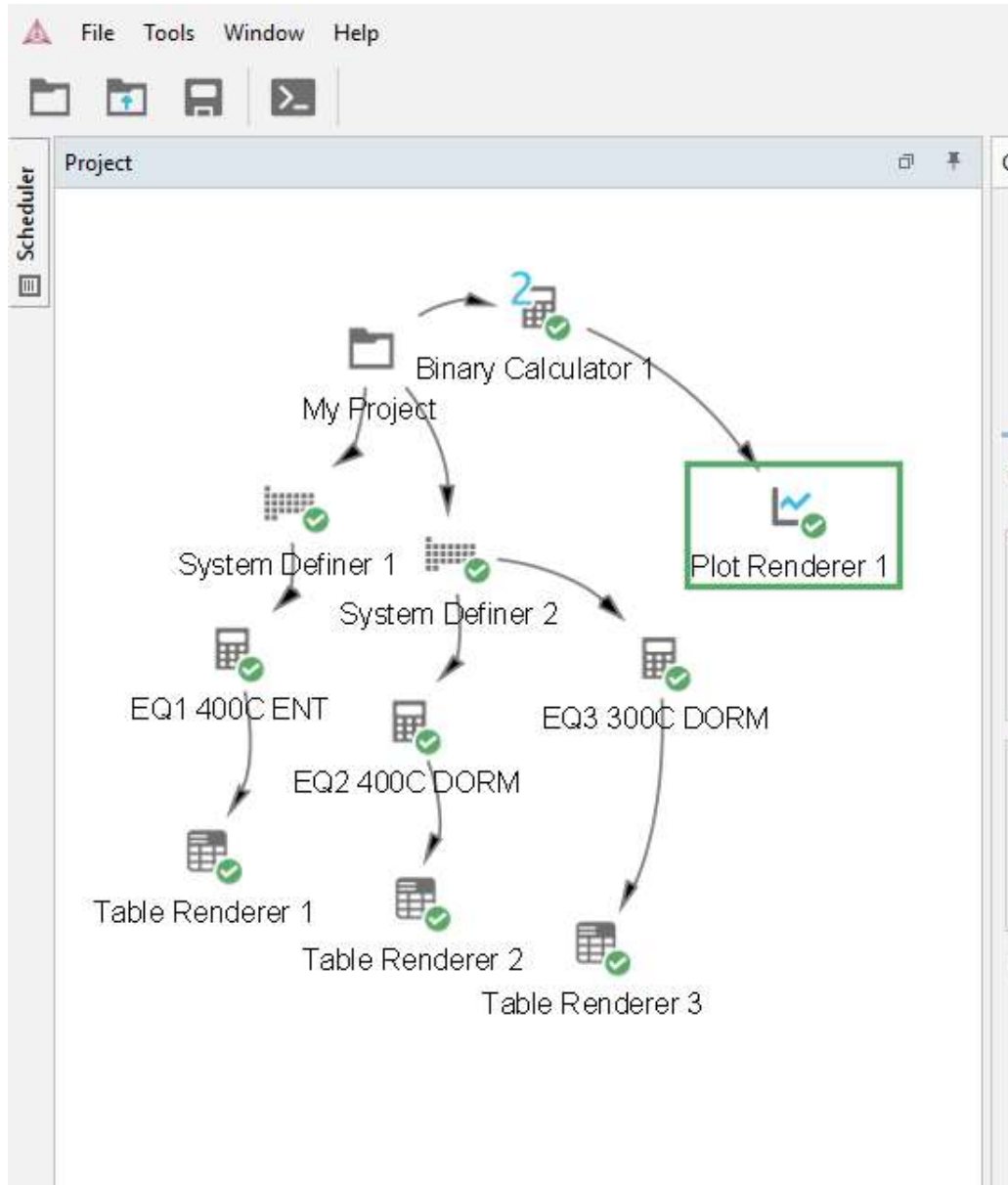


| Quantities                               |           |      |
|------------------------------------------|-----------|------|
| Temperature                              | 400.00000 | [°C] |
| Normalized driving force of AL2CU_C16    | 0.00000   |      |
| Normalized driving force of FCC_A1       | 0.00000   |      |
| Normalized driving force of THETA_DPRIME | -0.41589  |      |
| Normalized driving force of THETA_PRIME  | -0.22109  |      |
| System                                   |           |      |
| Moles                                    | 1.00000   |      |

$DGM(fcc) = DGM(Al_2Cu) = 0$  means the phase is stable and present in equilibrium.

Negative driving force (DGM) shows how far away from equilibrium the phase is. Multiply by  $RT$  to get a value, e.g.  $0.2211 \times 8.314 \times 673.15 = 1237.4 \text{ J/mol}$  for  $\theta'$

# Stable and metastable phases in Al-Cu



5. Clone the Project from Sys Def 1
6. Set all phases except FCC to status DORMANT
7. Calculate



## Quantities

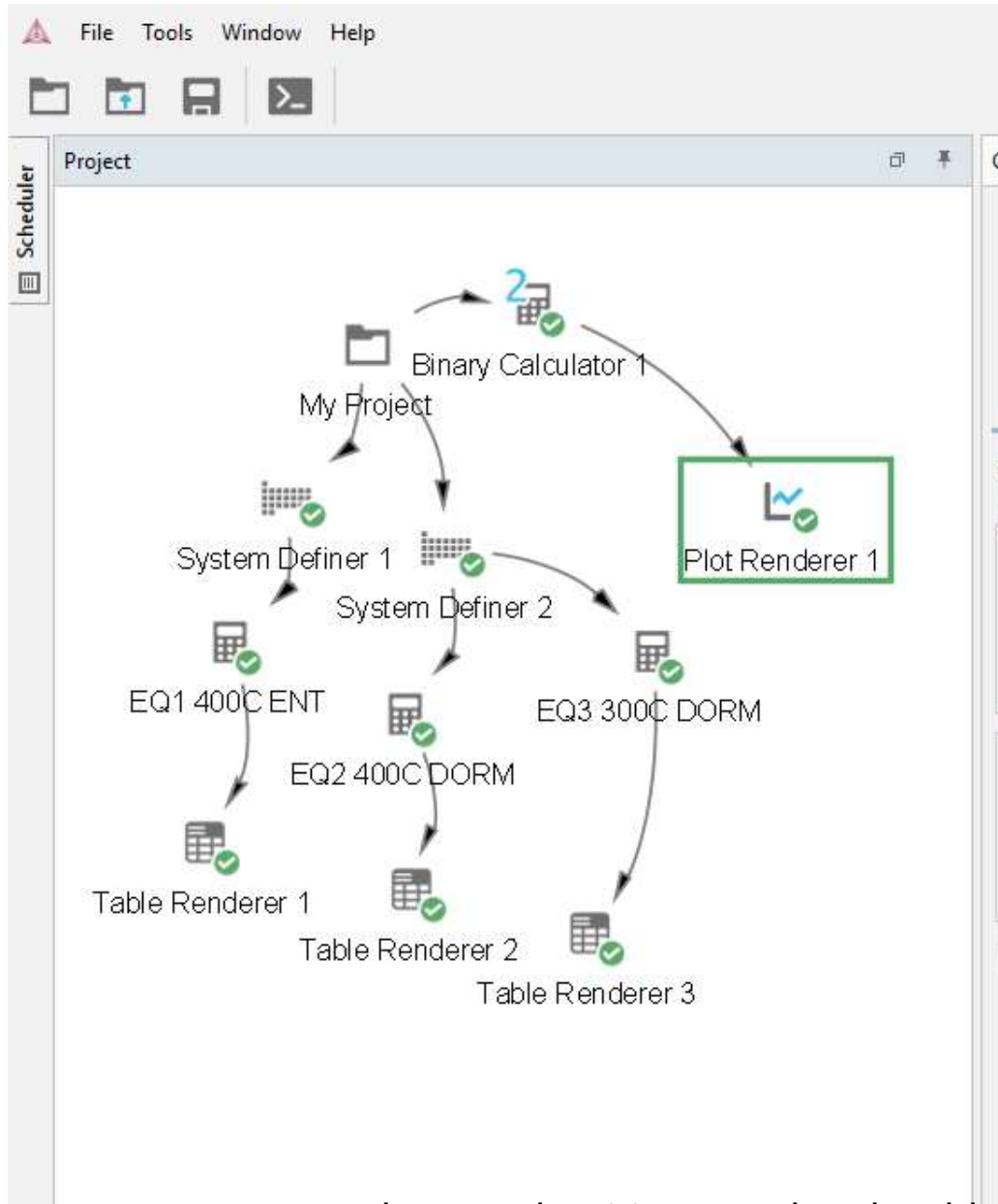
|                                          |           |
|------------------------------------------|-----------|
| Temperature                              | 400.00000 |
| Normalized driving force of AL2CU_C16    | 0.12013   |
| Normalized driving force of FCC_A1       | 0.00000   |
| Normalized driving force of THETA_DPRIME | -0.32520  |
| Normalized driving force of THETA_PRIME  | -0.09917  |

## System

|                    |              |
|--------------------|--------------|
| Moles              | 1.00000      |
| Mass               | 27.34764     |
| Temperature        | 673.15000    |
| Total Gibbs Energy | -24007.48294 |

Same temperature, but only FCC entered and stable. DGM change for the other phases: for Al<sub>2</sub>Cu it is now positive, meaning it should be stable if allowed. For  $\theta'$  and  $\theta''$  the value is less negative now, compared with this metastable single-phase FCC equilibrium.

# Stable and metastable phases in Al-Cu



8. Clone project tree from the previous Equilibrium calculator
9. Set T = 300 C. Calculate.



| Quantities                               |           |      |
|------------------------------------------|-----------|------|
| Temperature                              | 300.00000 | [°C] |
| Normalized driving force of AL2CU_C16    | 0.45267   |      |
| Normalized driving force of FCC_A1       | 0.00000   |      |
| Normalized driving force of THETA_DPRIME | -0.19275  |      |
| Normalized driving force of THETA_PRIME  | 0.10302   |      |
| System                                   |           |      |
| Moles                                    | 1.00000   |      |
| Mass                                     | 27.34764  | [g]  |

Lower temperature here, only FCC entered and stable. DGM changes for the other phases: now it is positive for both Al<sub>2</sub>Cu and  $\theta'$ .

Zoom meeting has the same contact details as today.

Course will start the same time, 09:00 CET (Berlin/Stockholm)

# End of Day 2