The role of CALPHAD based tools in an ICME Modeling Infrastructure

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Introduction

The 2008 National Academies report on Integrated Computational Materials Engineering (ICME) and President Obama's announcement of the Materials Genome Initiative (MGI) in June 2011 highlights the growing interest in using computational methods to aid materials design and process improvement.

For more than 20 years CALPHAD (CALculation of PHAse Diagrams) based tools have been used to accelerate alloy design and improve processes. CALPHAD is based on relating the underlying thermodynamics of a system to predict the phases that can form and the amounts and compositions of those phases in multicomponent systems of industrial relevance.

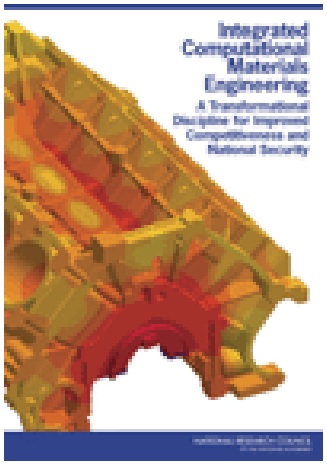
The goal of this presentation is to illustrate:

1. How CALPHAD is an integral part of the foundation of an ICME / Materials Design infrastucture

2. The broad range of applications and problems in the materials life cycle that CALPHAD based tools can be used to investigate

What is ICME?

Thermo-Calc Software



The National Academies Press, 2008

Integrated Computational Materials Engineering: A Transformational Discipline for Improved Competitiveness and National Security

ICME: an approach to design products, the materials that comprise them, and their associated materials processing methods by linking materials models at multiple length scales. Key words are "Integrated", involving integrating models at multiple length scales, and "Engineering", signifying industrial utility.

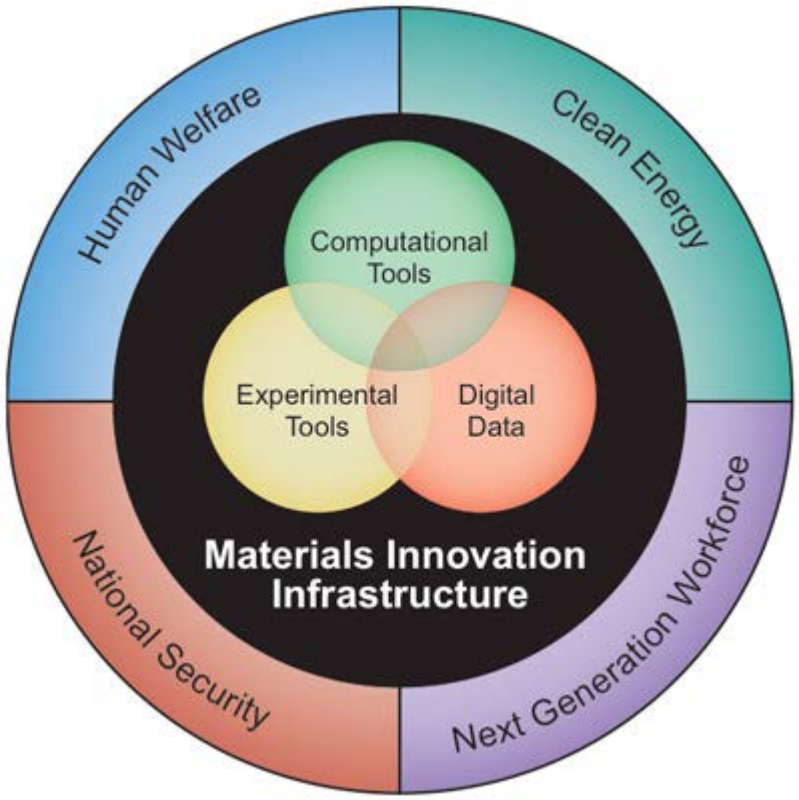
Focus is on the materials, i.e. understanding how processes produce material structures, how those structures give rise to material properties, and how to select materials for a given application. This report describes the need for using multiscale materials modeling to capture the process-structures-properties-performance of a material.

What is MGI?

June 2011

Materials Genome Initiative for global competitiveness

The Materials Genome Initiative is a national initiative to double the speed and reduce the cost of discovering, developing, and deploying new advanced materials.



What should be modeled in the ICME and MGI?

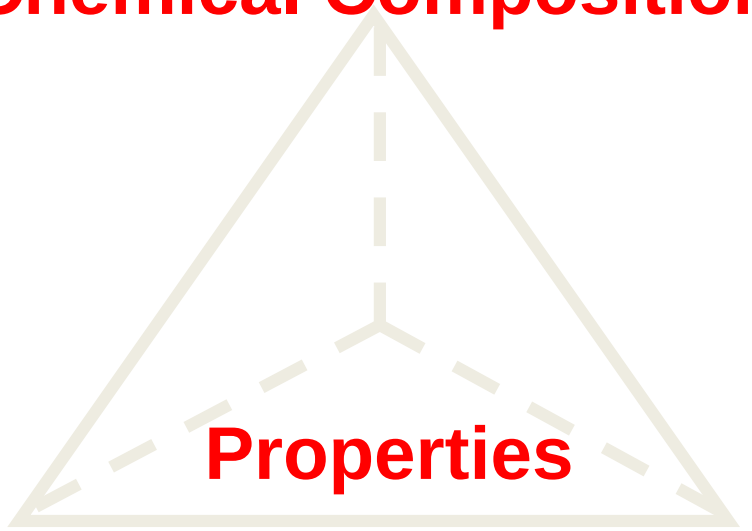
The analogy of a materials genome to a human genome implies that something of the nature of the material is encoded in the chemical composition of a material and that we should be able to read this.

But nurture is important, as well as nature, and to extend the analogy further, nurture is the equivalent of processing the material.

In ICME/MGI we are striving to model how the structure and properties of a material are affected by its composition, synthesis, processing and usage.

Modelling of structure evolution and kinetic processes thus depends on what models are available for structure-property relations.

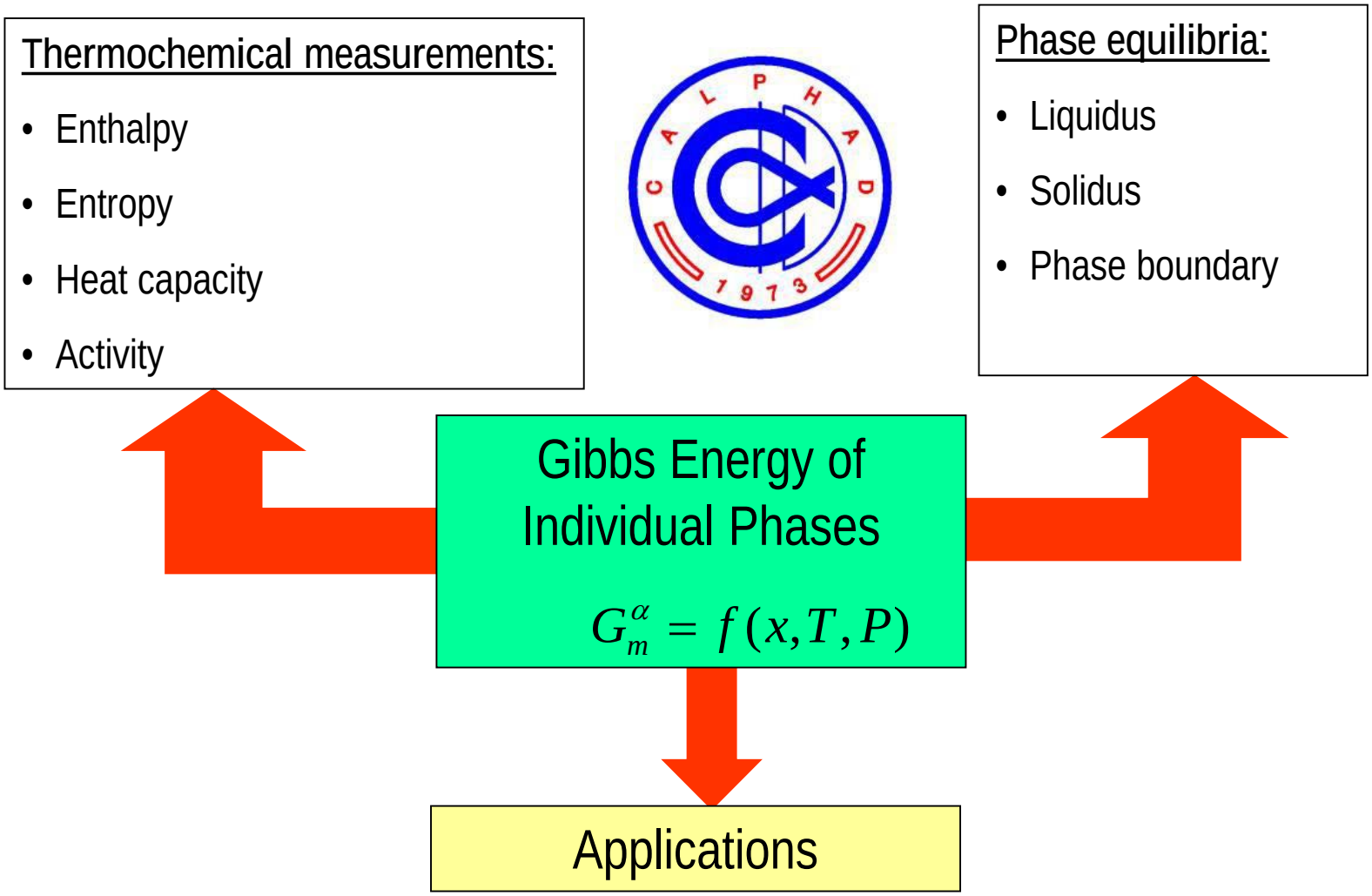
The influence of chemistry on microstructure and properties



Heat treating can best be defined as “the controlled application of time, temperature and atmosphere to produce a predictable change in the internal structure (i.e. the microstructure) of a material.” Dan Herring, 100th Column of the “Heat Treat Doctor” published in Industrial Heating magazine

What is CALPHAD

Thermo-Calc Software



A phase based approach to modeling the underlying thermodynamics and phase equilibria of a system through a self consistent framework that allows extrapolation to multicomponent systems.

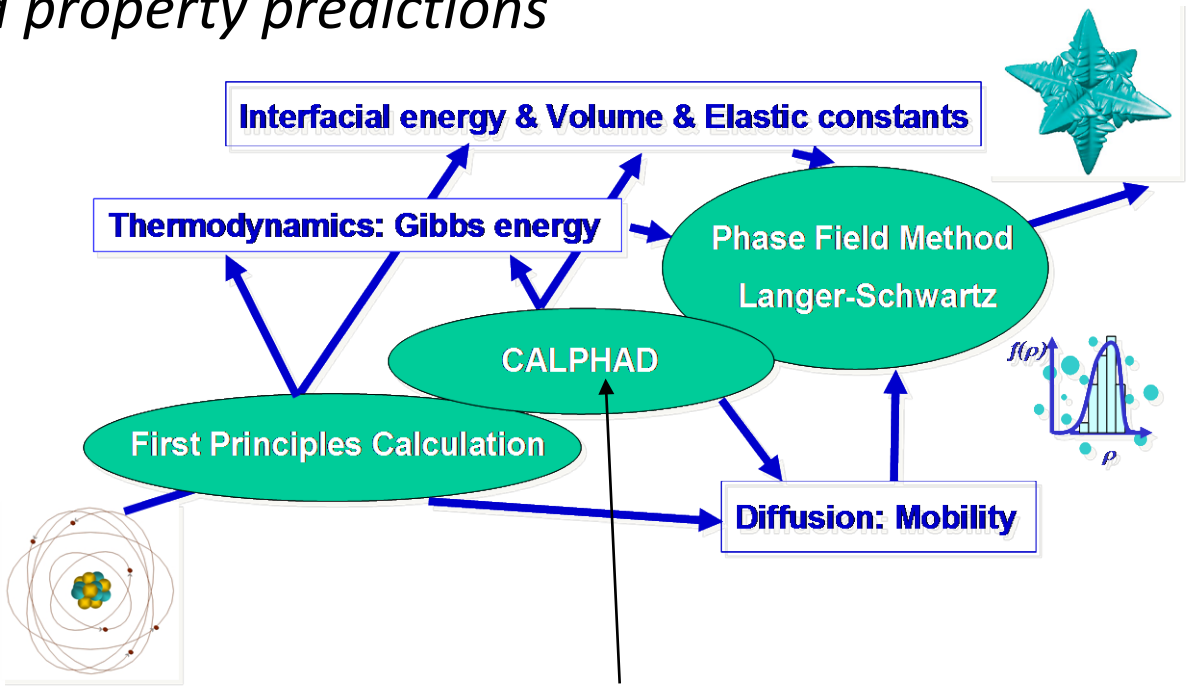
CALPHAD – an important bridge

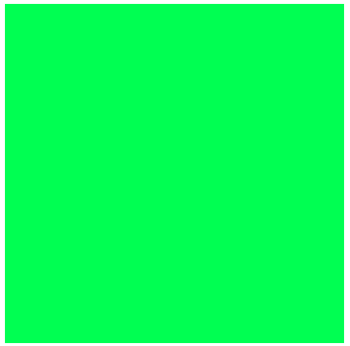
Linking atomistic to multicomponent

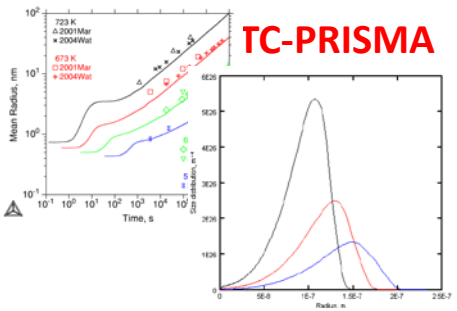
Linking thermodynamics and kinetics

A bridge to microstructural evolution and property predictions

Microstructure evolution and material properties

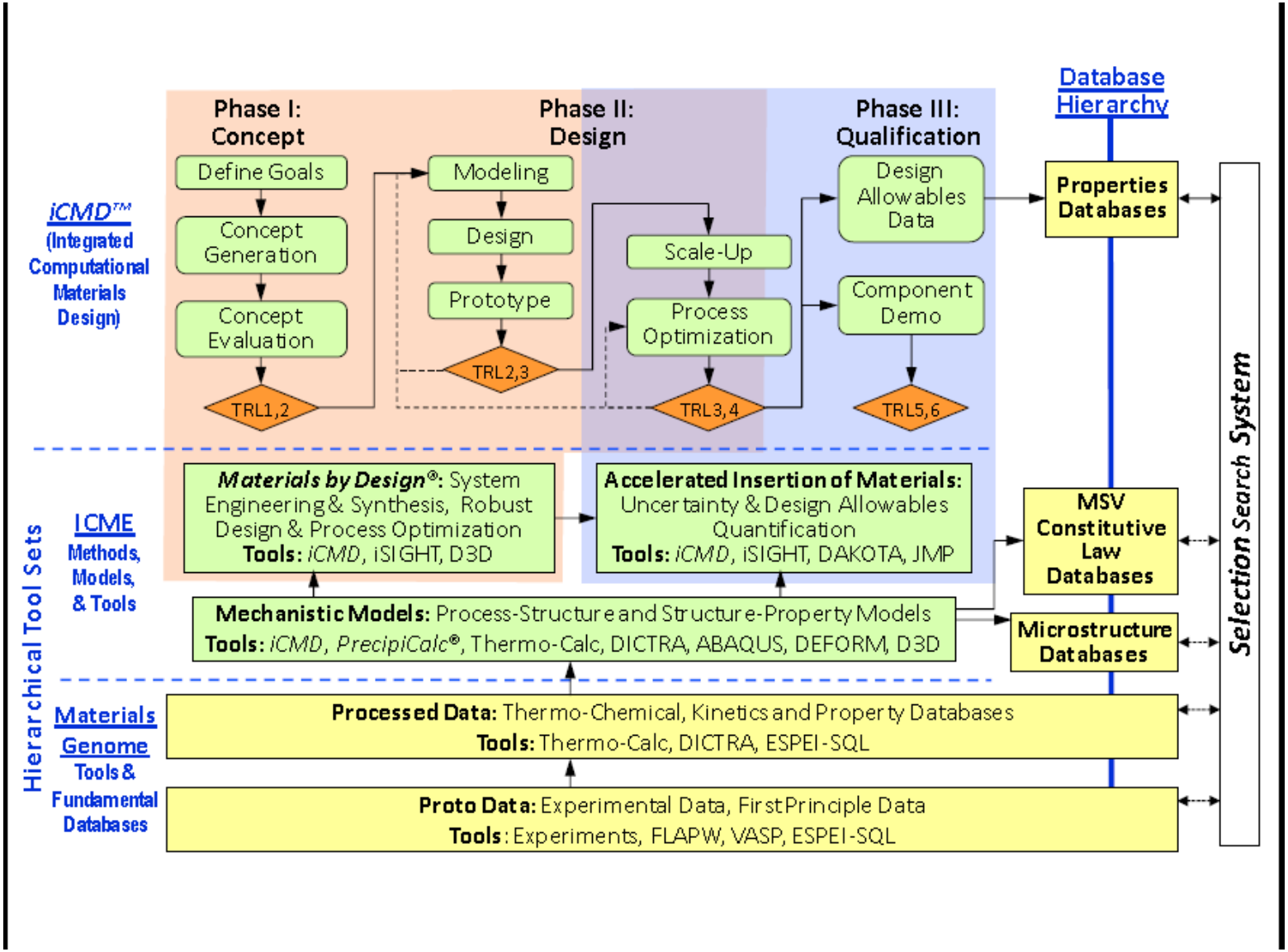






The development of consistent databases where each phase is described separately using models based on physical principles and parameters assessed from experimental data is a key.

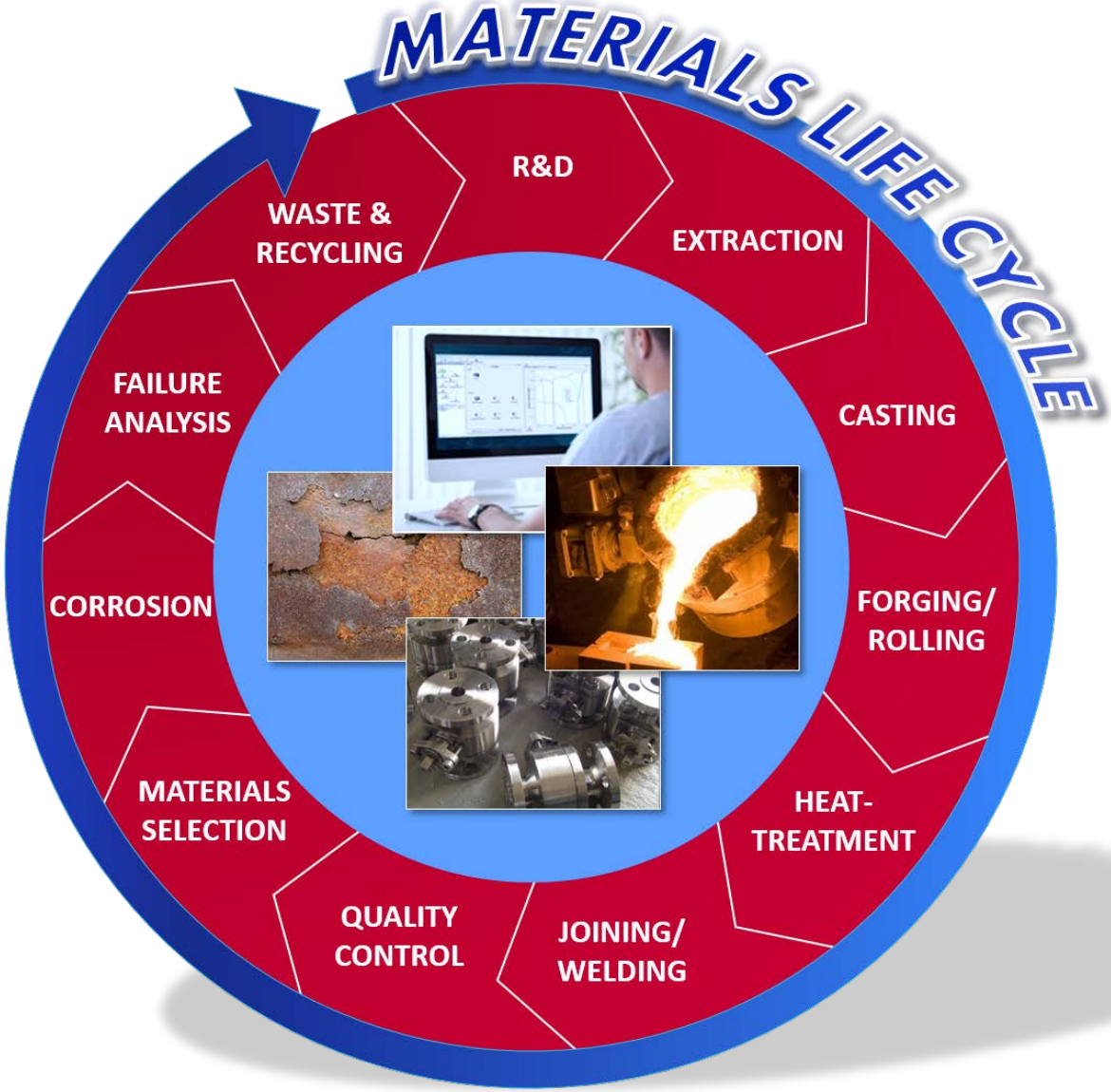
CALPHAD – a foundation of MGI, ICME and ICMD



Slide courtesy of Prof. G. Olson, Northwestern University, QuesTek Innovations LLC

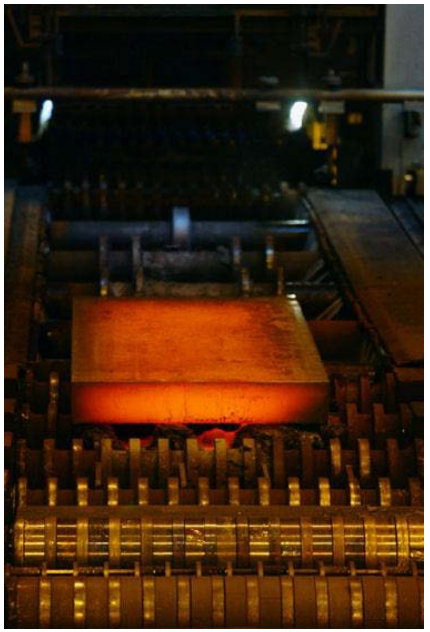
Application to the materials life cycle

Thermo-Calc Software



CALPHAD based software: Thermo-Calc

- Calculating stable and meta-stable heterogeneous phase equilibrium
- Amount and composition of phases
- Transformation temperatures, e.g. liquidus and solidus temperature
- Predicting driving forces for phase transformations
- Phase diagrams (binary, ternary, isothermal, isoplethal, etc.)
- Molar volume, density and thermal expansion
- Scheil-Gulliver (non-equilibrium) solidification simulations
- Thermochemical data such as;
  - enthalpies
  - heat capacity,
  - activities, etc.
- Thermodynamic properties of chemical reactions
- **And much, much more….**



- Designing and optimization of alloys
- Design and optimization of processes

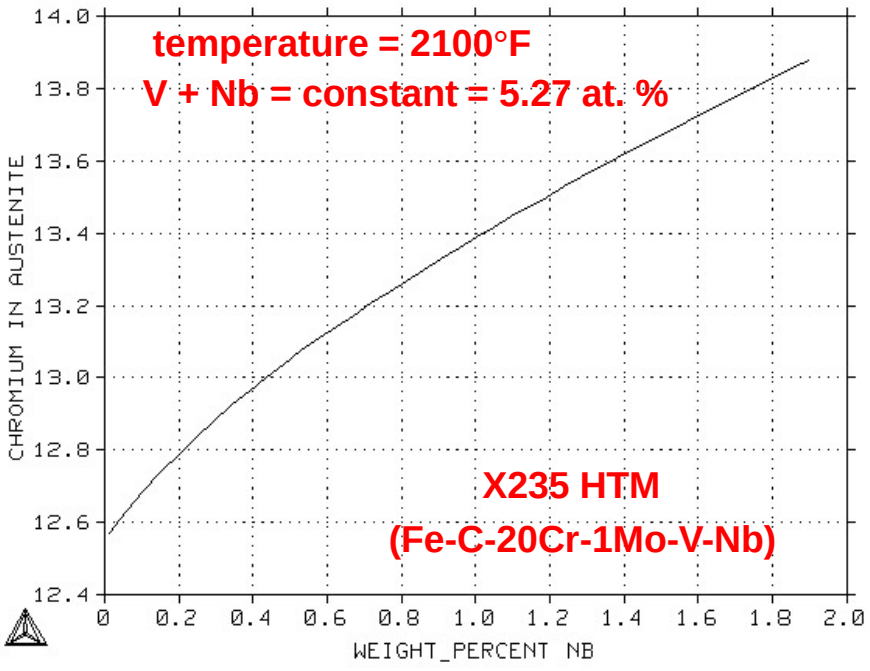
Early example using thermodynamic calcs in alloy design

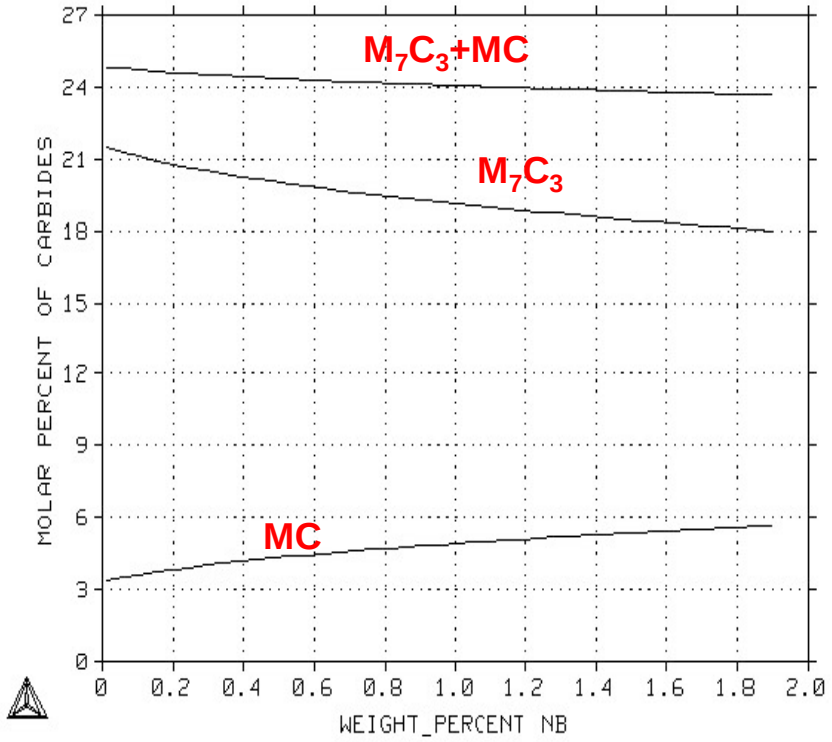
- The first systematic use of of Calphad computational tools and databases for industrial purposes. Based only on equilibrium calculations.
- In 1983 Swedish steel producer Sandvik developed a new generation of duplex stainless steels.
  - –Same price level as the conventional 18/8 steel
  - –Twice the strength
  - –Better corrosion resistance
  - –Reduced experimental costs (2 instead of 10 years)
- Most important to have 50/50 mixture of FCC-BCC.
- Avoid TCP (e.g. sigma phase)
- Same PRE-number in both phases. PRE (Pitting Resistance Equivalent) calculated empirically from phase composition.

Slide courtesy of Prof. J. Ågren, KTH

Example: Influence of alloy composition

Example provided by Alojz Kajinic, Crucible Research (ATI Powder).



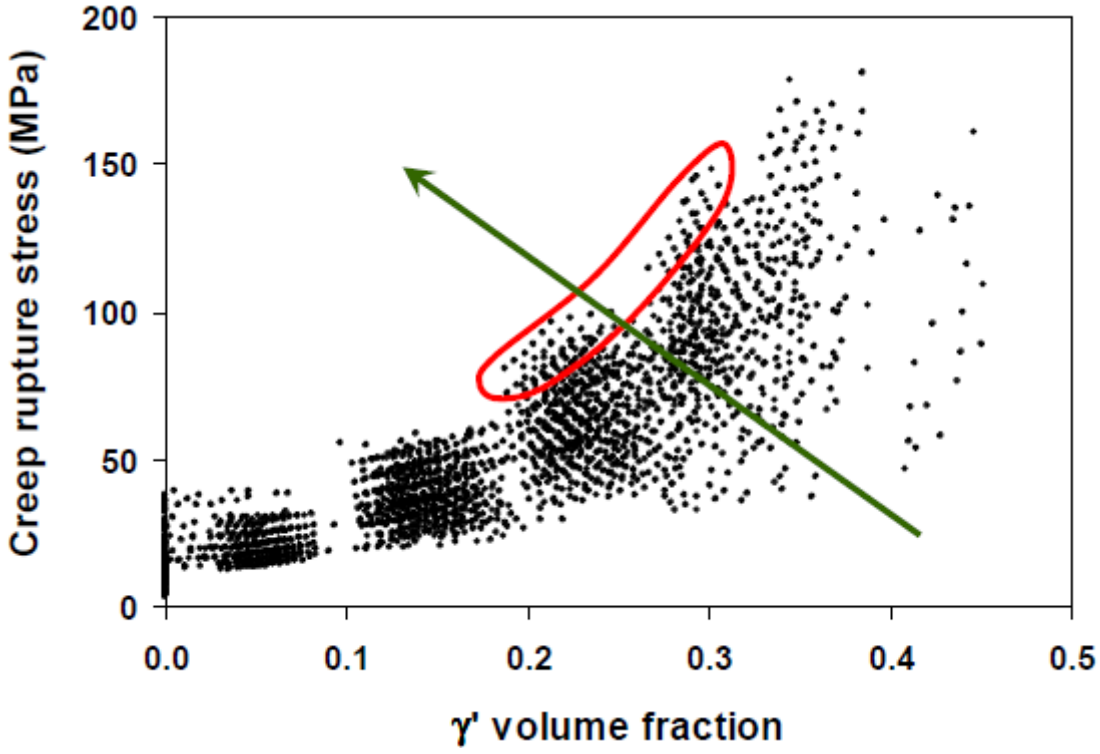


Example: Optimization of an alloy composition

Thermo-Calc Software

Franck Tancret – Université de Nantes (TMS 2009):

Optimization of an alloy composition for the design of weldable and creep resistant superalloys using Matlab, TC-Matlab toolbox and neural net models. Over 16,000 compositions assessed.



TCNI5 – Binary evaluations

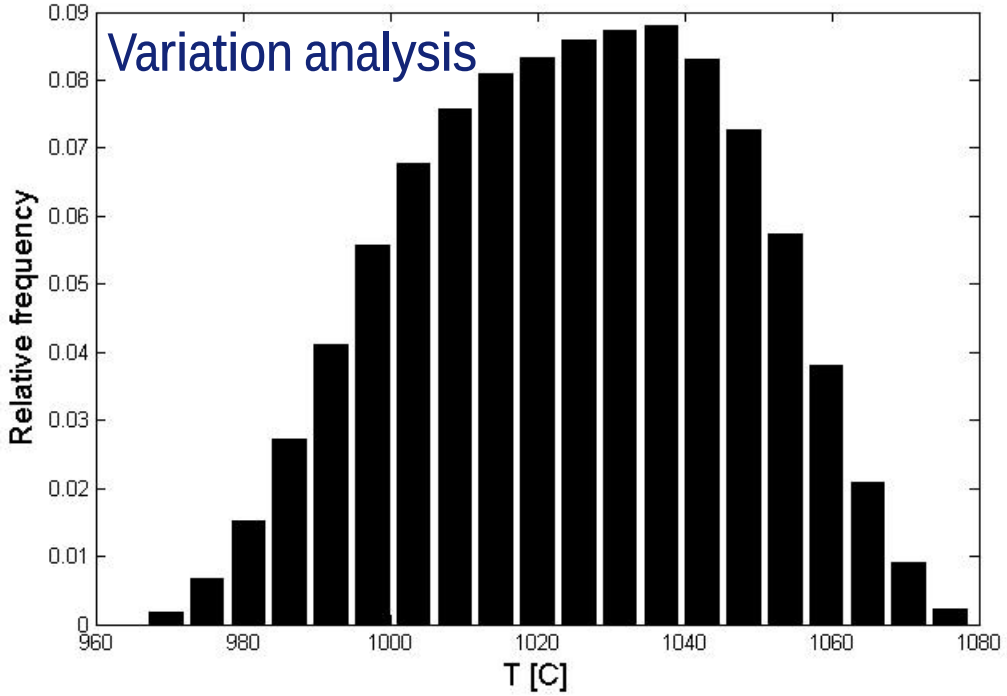
Thermo-Calc Software

	Al	B	C	Co	Cr	Fe	Hf	Mo	N	Nb	Ni	Pd	Pt	Re	Si	Ta	Ti	V	W
B	x																		
C	x	x																	
Co	x	x	x																
Cr	x	x	x	x															
Fe	x	x	x	x	x														
Hf	x	x	x	x	x	x													
Mo	x	x	x	x	x	x	x												
N	x	x		x	x	x		x											
Nb	x	x	x	x	x	x	x	x	x										
Ni	x	x	x	x	x	x	x	x	x	x									
Pd	x	x	x	x	x	x	x	x		x	x								
Pt	x	x	x	x	x	x	x			x	x	x							
Re	x	x	x	x	x	x	x	x		x	x	x	x						
Si	x	x	x	x	x	x	x	x	x	x	x	x	x	x					
Ta	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x				
Ti	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x			
V	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x		
W	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	
Zr	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x

- 20 + 3 elements.
- 184 of 190 binary systems assessed for full range composition
- All Ni containing ternaries plus other ternary systems also assessed to full range of composition (184 in total)
- 292 intermetallic and solution phases

Example: Variation of properties within specification tolerances

SAF 2507: Fe – 25% Cr – 7% Ni – 4% Mo – 0.27% N – 0.02% C. Sigma phase is predicted to be stable below 1030 ºC. How is this temperature influenced by changes in the alloy chemistry?



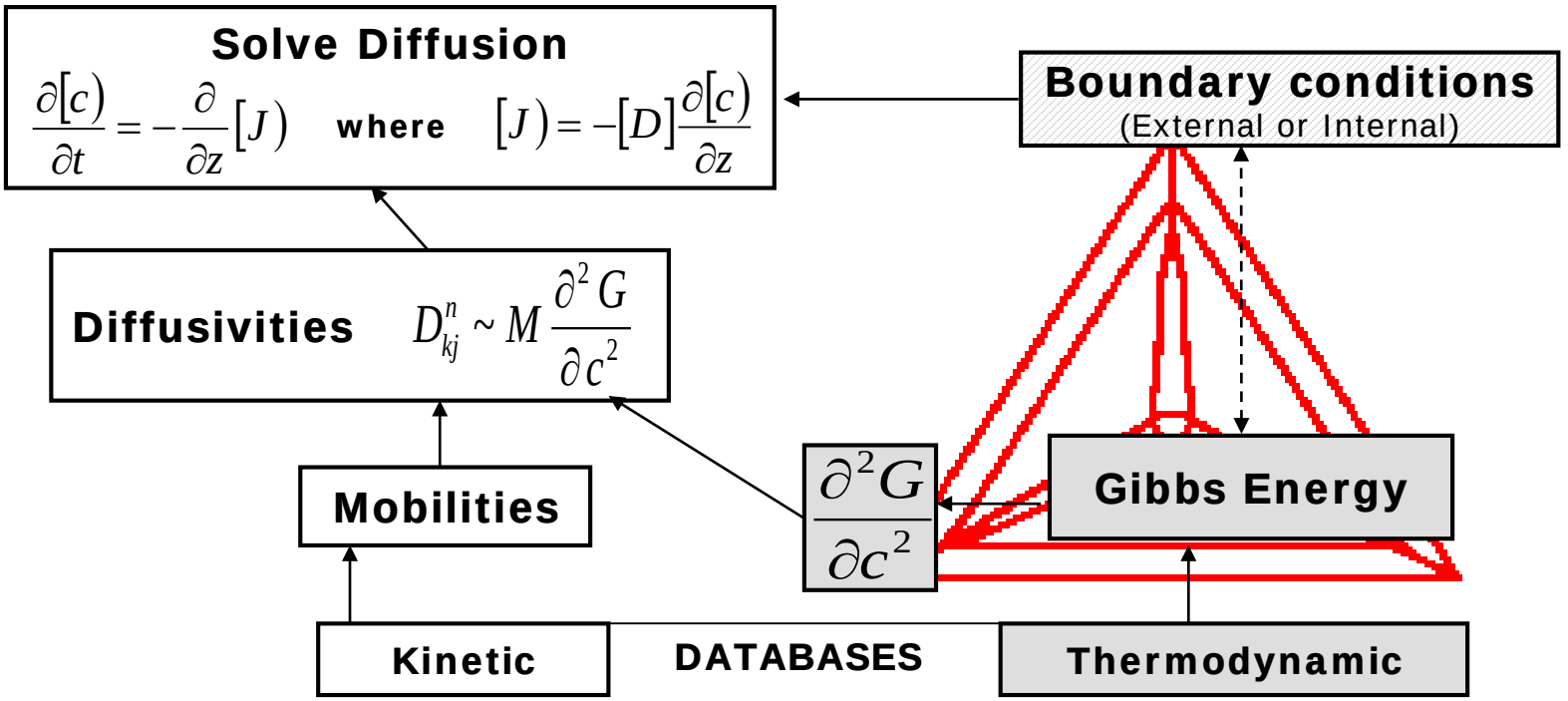
Composition range:

Fe	Base
Cr	23 – 27%
Ni	6 – 8%
Mo	3 – 5%
N	0.25 – 0.29%
C	0 – 0.03%

12^5 = 248832 calculations

CALPHAD based software: DICTRA

A general software package for simulation of **Di**ffusion **C**ontrolled **TRA**nsformations in multi component alloys.



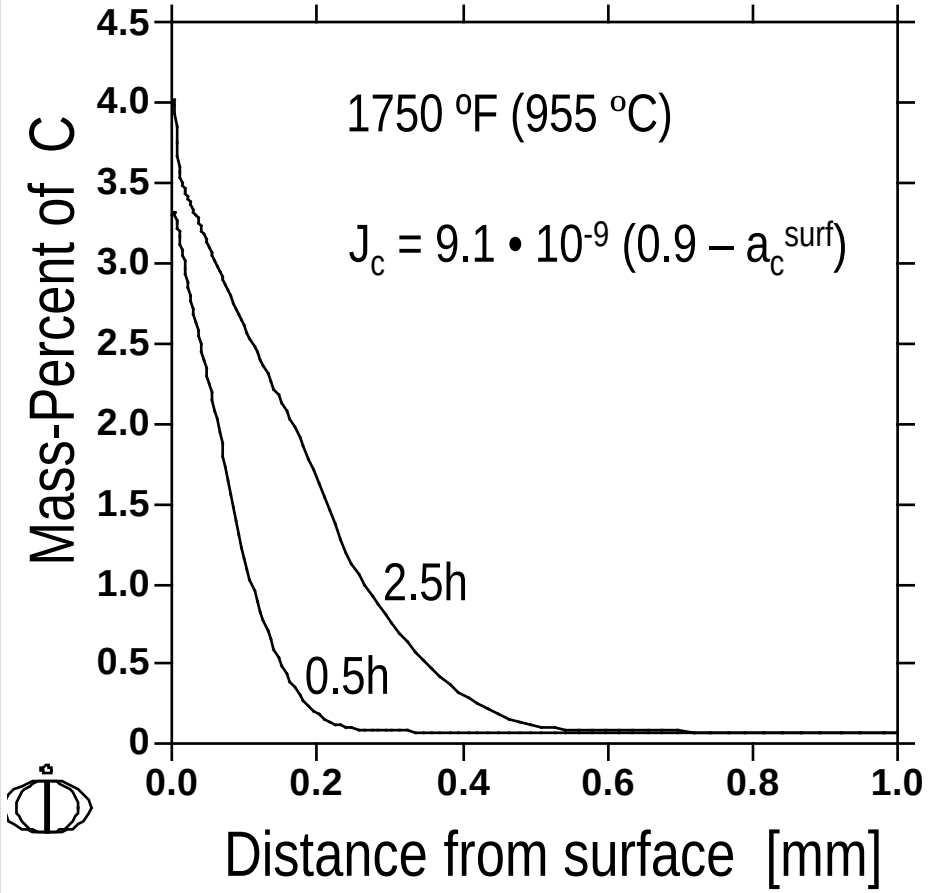
All simulations depend on assessed kinetic and thermodynamic data.

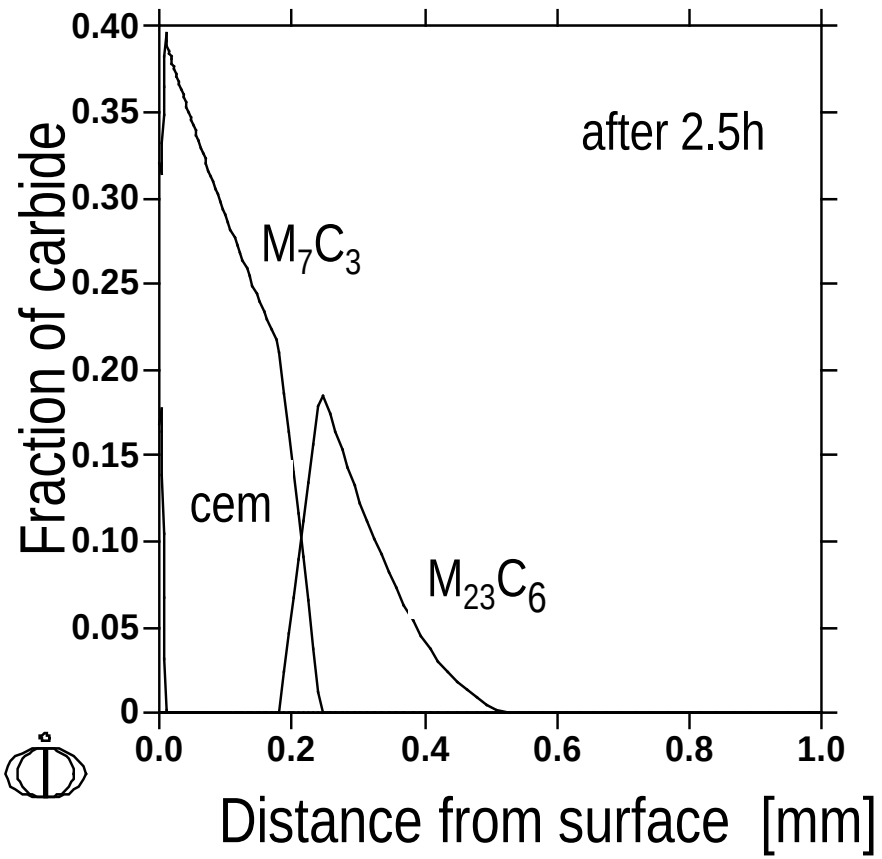
A numerical finite difference scheme is used for solving a system of coupled parabolic partial differential equations.

Example: Fe-13Cr-5Co-3Ni-2Mo-0.07C

Thermo-Calc Software

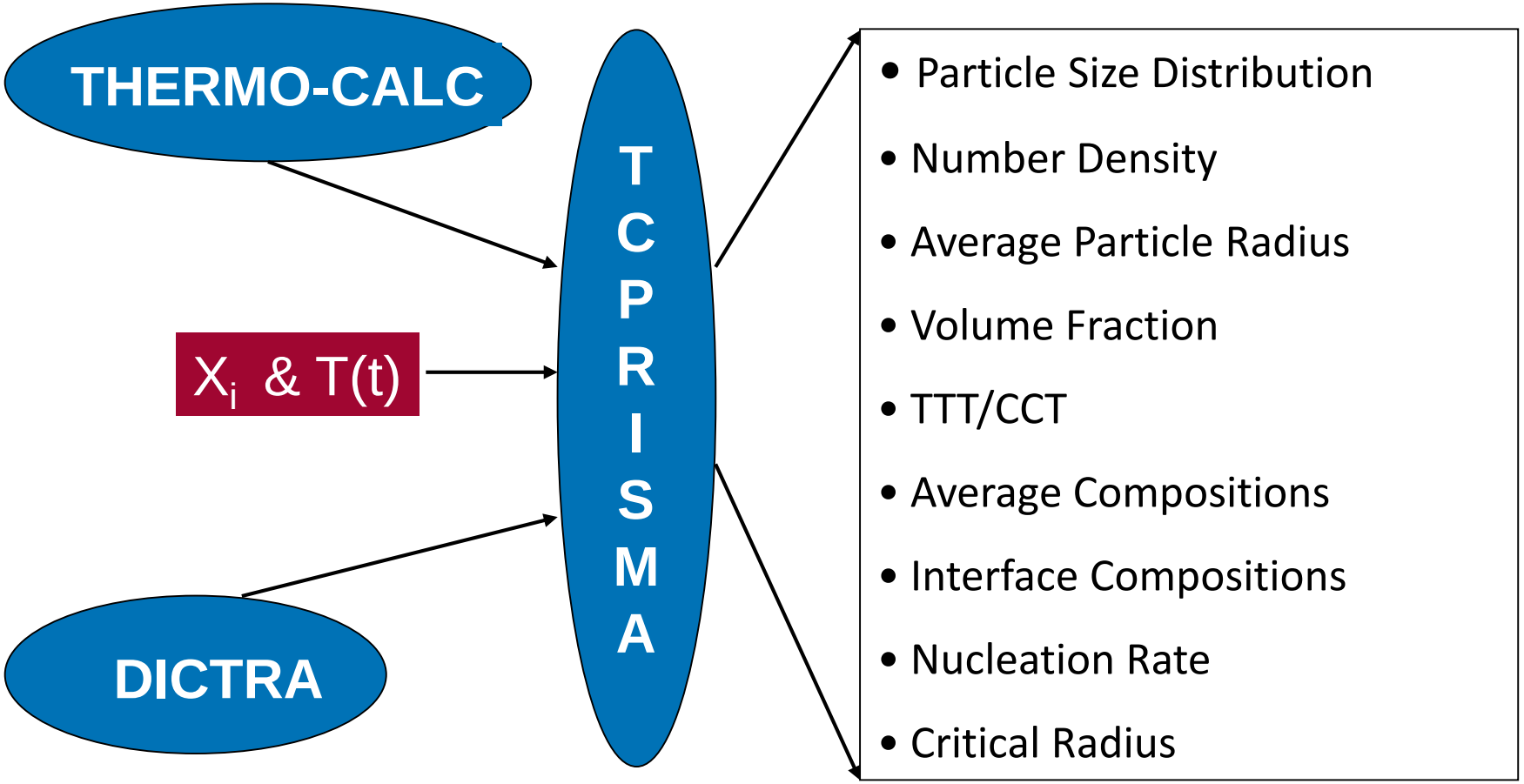
An example involving a complex alloy where alloying elements will tend to form carbides at high C-activities.



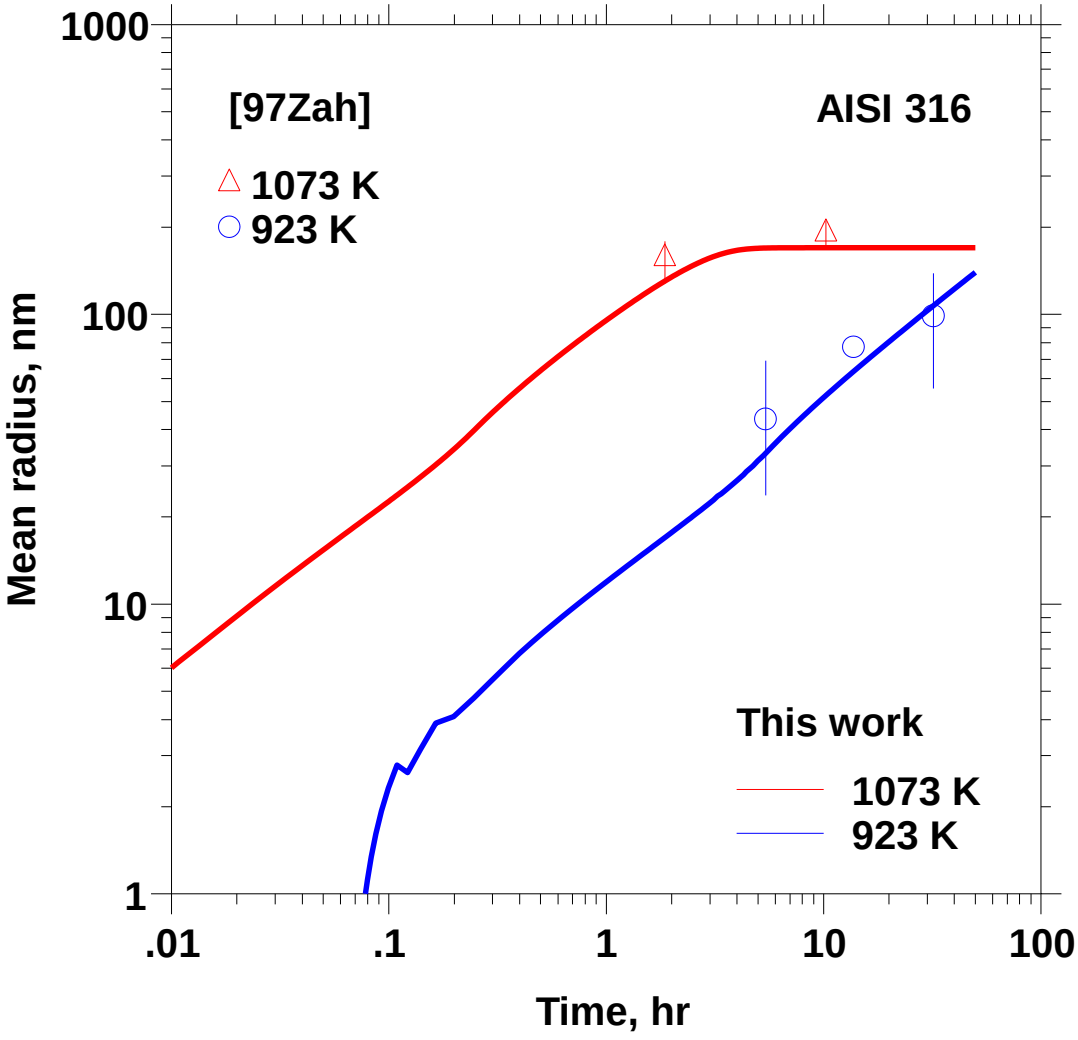


CALPHAD based software: TC-PRISMA

Concurrent nucleation, growth/dissolution, coarsening using a mean field approach.



Example: Precipitation kinetics M23C6 in AISI 316



Input data for simulation:

- Composition
  - C 0,08%
  - Cr 18%
  - Ni 12%
  - Mo 2%
  - Mn 1.5%
- Time & temperture
- Nucleation at grainboundaries

@ 650 °C

- γ-grainsize =100 μm
- σ = 0.3 J/m^2

@ 800 °C

- γ-grainsize =1000 μm
- σ = 0.2 J/m^2

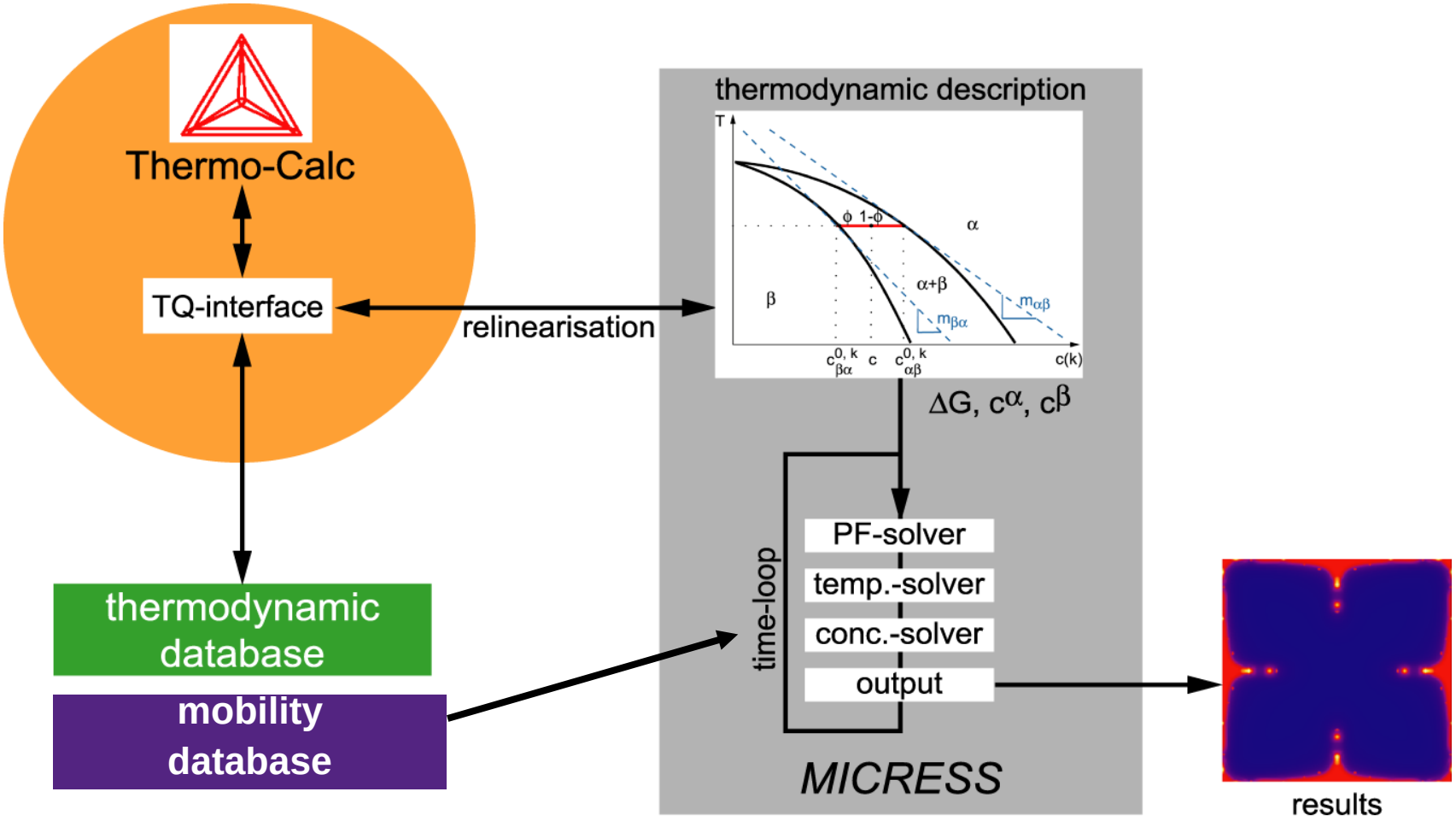
CALPHAD based software: Phase field

- Output:
  - Detailed morphology
  - Concentration fields
  - Stress fields
  - Plastic strain fields (dislocation density fields)
  - ...
- Need or can use input from
  - Multicomponent thermodynamics
  - Multicomponent diffusion analysis
  - Interfacial energy and mobility
  - Elastic coefficients and stresses
  - Stress-free transformation strain tensor (eigen strains)
  - Plastic relaxation
  - Fluid flow (Navier Stokes)
  - ....

Slide courtesy of Prof. J. Ågren, KTH

CALPHAD Based Software: Phase field

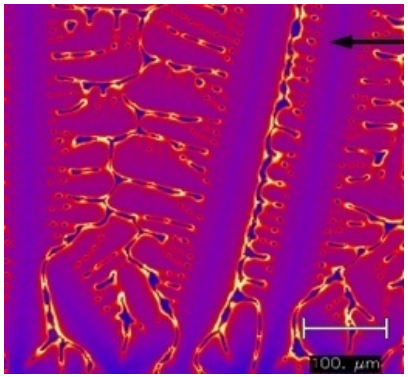
Slide Courtesy of G. Schmitz, Access



MICRESS Simulations of technical alloy grades

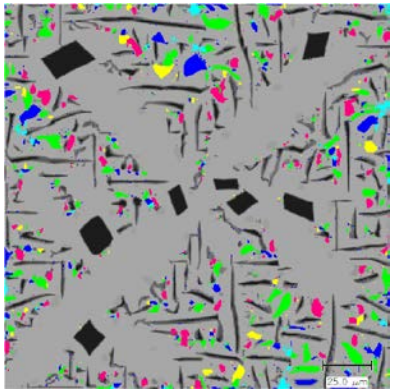
Thermo-Calc Software

Slide Courtesy of G. Schmitz, Access



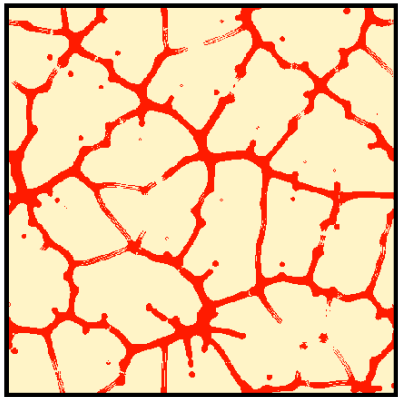
Steel
(e.g. stainless steel)

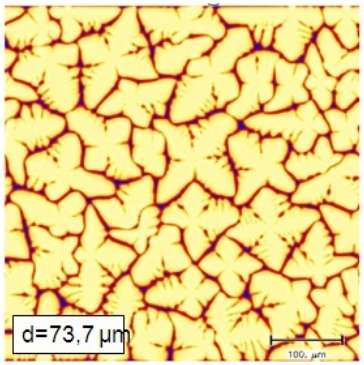
Al-alloys
(e.g. KS 1295)



cast iron
(e.g. GJS)

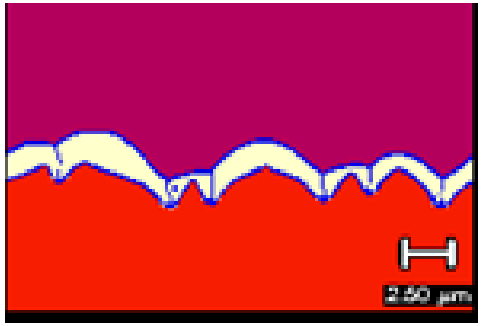
Mg-alloys
(e.g. AZ 91)





Superalloys
(e.g. IN 718)

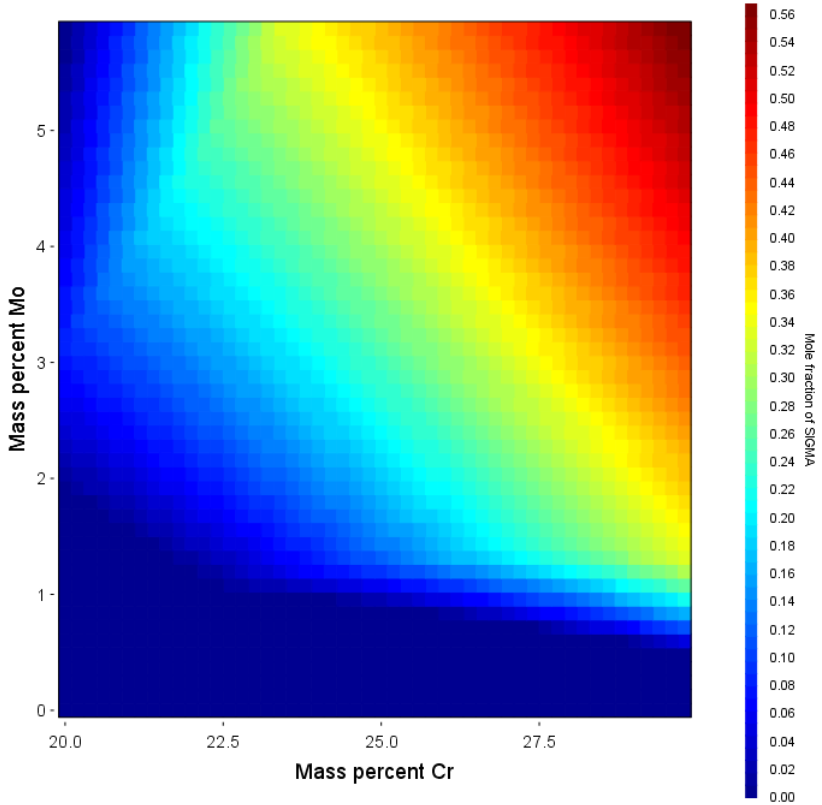
Solders
(e.g. SAC)

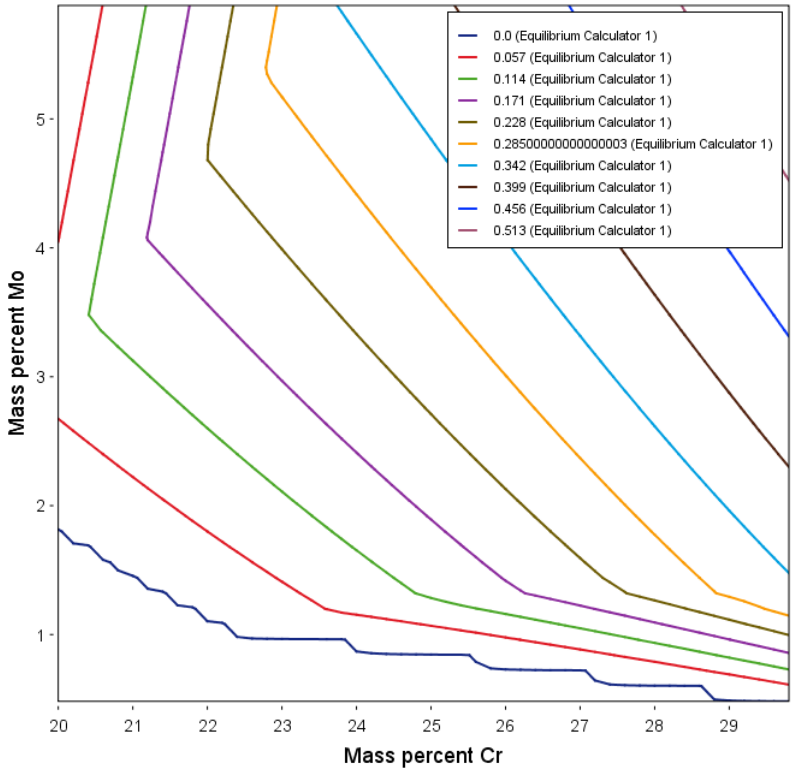


Visualizing data in new ways – property maps

Thermo-Calc Software

Thermo-Calc 4.1: “Property grid” calculation type has been added.

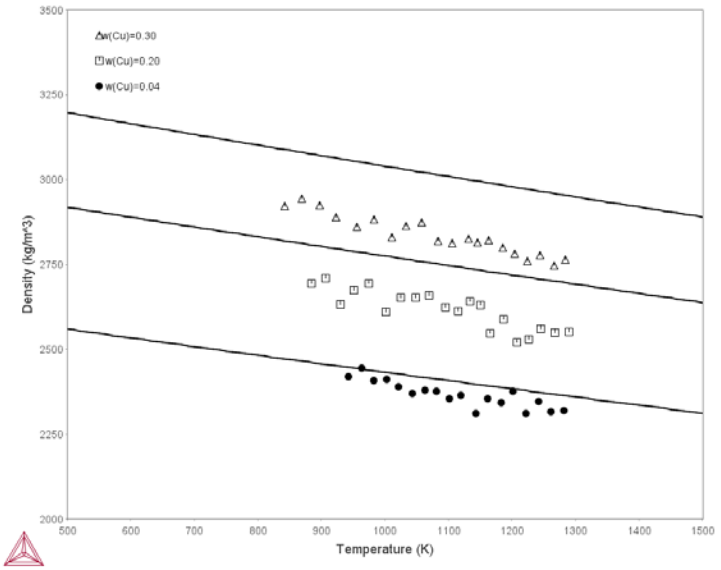


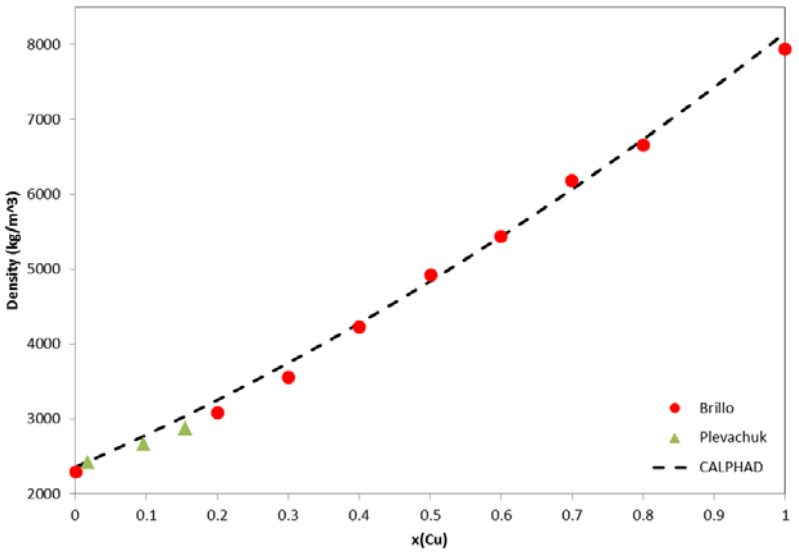


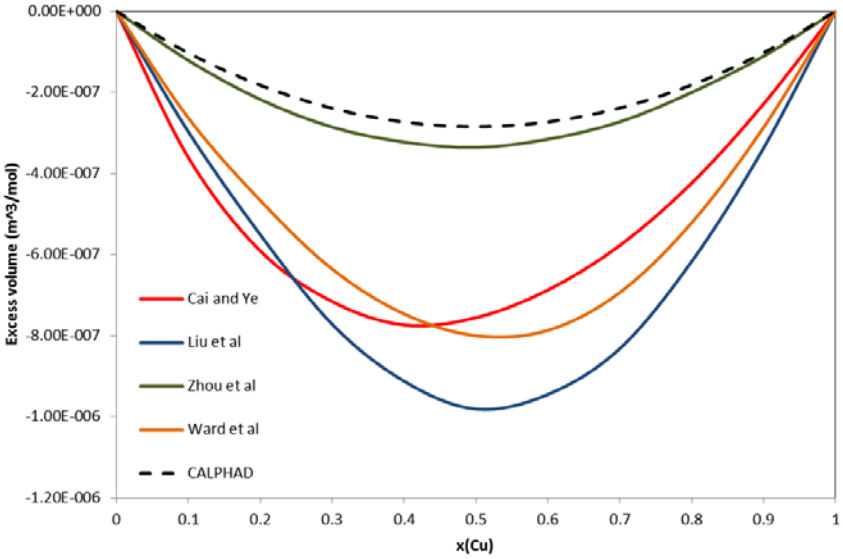
Molar Volume of Liquid $Al_{1-x}Cu_x$

- CALPHAD assessment of the molar volume of liquid Al-Cu alloys is based on following experimental data
  - Plevachuk et al (Metal Trans 39A, 3040, 2008)
  - Brillo et al (Int J Mater Res 99, 162, 2008)
- Fitting to the experimental data by Plevachuk et al gives a positive excess volume
- Fitting to the data by Brillo et al gives a negative excess volume
- It is impossible to simultaneously fit both sets of data
- Question: Which set of experimental data should we trust?

Case I

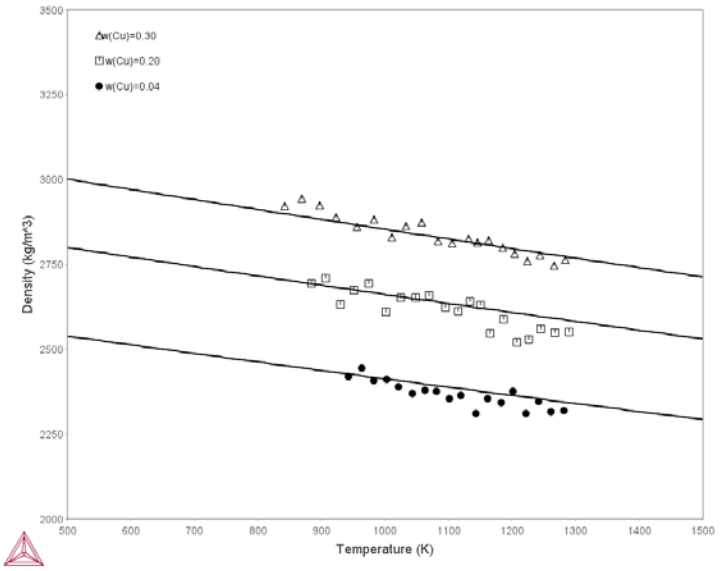


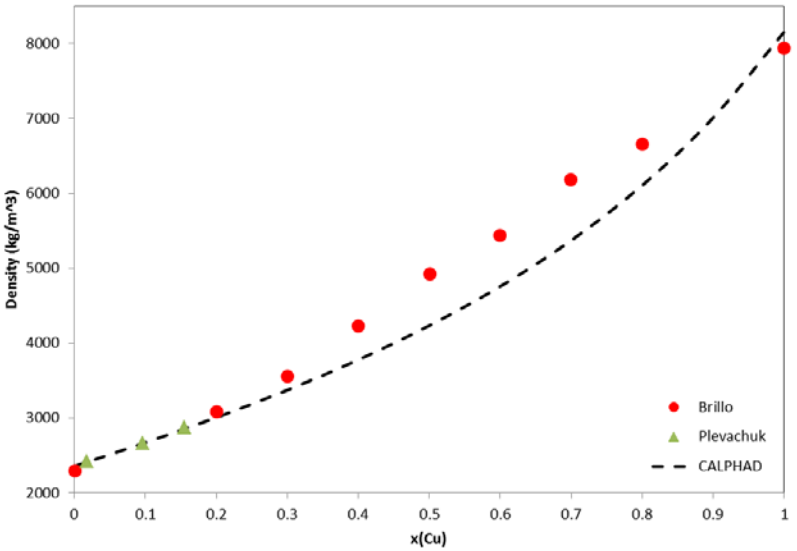


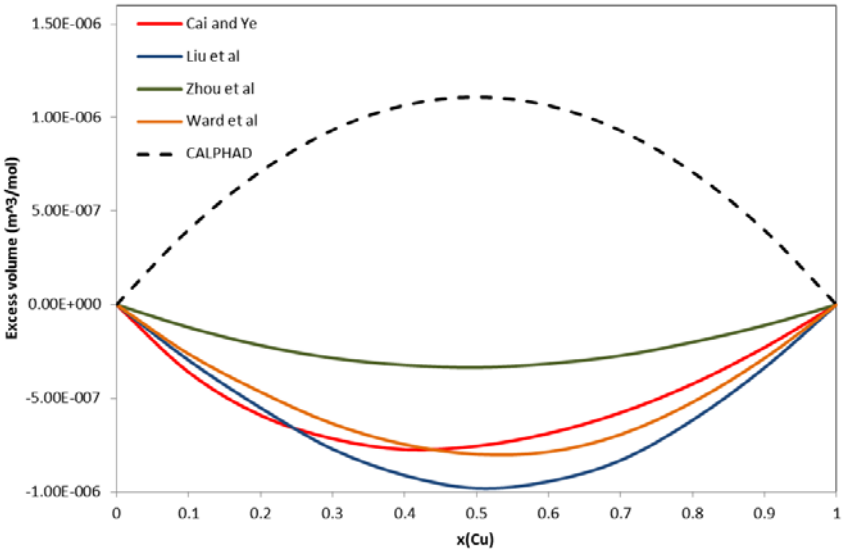


Fitting to the data by Brillo et al gives a negative excess volume, in qualitative agreement with MD simulations.

Case II







Fitting to the data by Plevachuk et al gives a positive excess volume, which contradicts MD results for the liquid Al-Cu alloy. Therefore, it is suggested that the experimental data from Brillo et al. be used for CALPHAD assessment.

Microstructure evolution, properties and beyond

Thermo-Calc Software

Coupling CALPHAD to macroscopic is not new:

ESI linked to CALPHAD databases in the 1990's with PRE-CAST

Questek built a design based platform based around CALPHAD models and tools

CALPHAD tools have been linked to CFD

Property predictions based on semi-empirical models also not new:

e.g. JMATPRO

But coupling in real-time, property predictions to kinetic models is still a goal.

Also, while there are many examples of validation of the CALPHAD approach more work is needed on how to predict uncertainties based around a prediction.

Summary

An important part of ICME and the MGI is aimed at improving our ability to model how processes produce material structures, how those structures give rise to material properties, and how to select materials for a given application in order to design and make better materials cheaper and faster. This requires multiscale materials models to capture the process-structures-properties-performance of a material.

CALPHAD is a phase based approach to modeling the underlying thermodynamics and phase equilibria of a system through a self consistent framework that allows extrapolation to multicomponent systems. The approach has also been extended to consider multicomponent diffusion as well. CALPHAD provides an important foundation to ICME and the MGI in a framework that is scalable to multicomponent systems of interest to industry.

Thermo-Calc Software

Questions?