

*The application of CALPHAD based  
tools to the Materials Genome  
Initiative and ICME*

Paul Mason

Thermo-Calc Software Inc.  
4160 Washington Road, Suite 230  
McMurray, PA 15317

# Goals of this lecture

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 30 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.

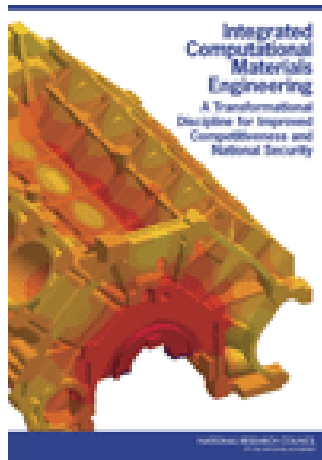
During this lecture, you will:

- Discover how CALPHAD relates to ICME and MGI
- Learn about the underlying concepts of the CALPHAD approach
- See how CALPHAD-based computational tools may be applied in the materials life cycle for a range of different materials.

There are three main sections to this lecture:

1. Describing what ICME, MGI and CALPHAD are and how CALPHAD fits into the larger ICME and MGI framework
2. A more detailed description of CALPHAD, CALPHAD based software tools and databases that underpin them.
3. Some practical examples of applications to the materials life cycle.

# What is ICME?



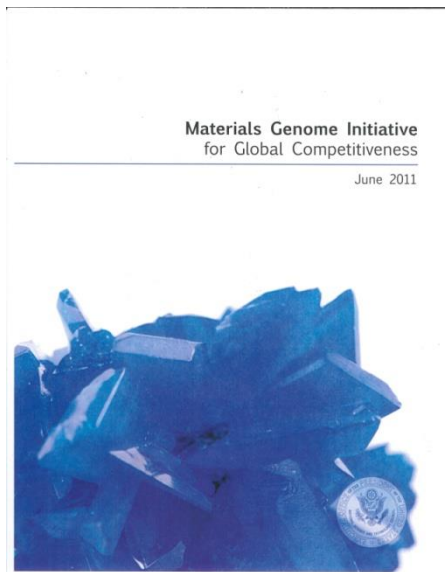
**The National Academies Press, 2008**

## **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.

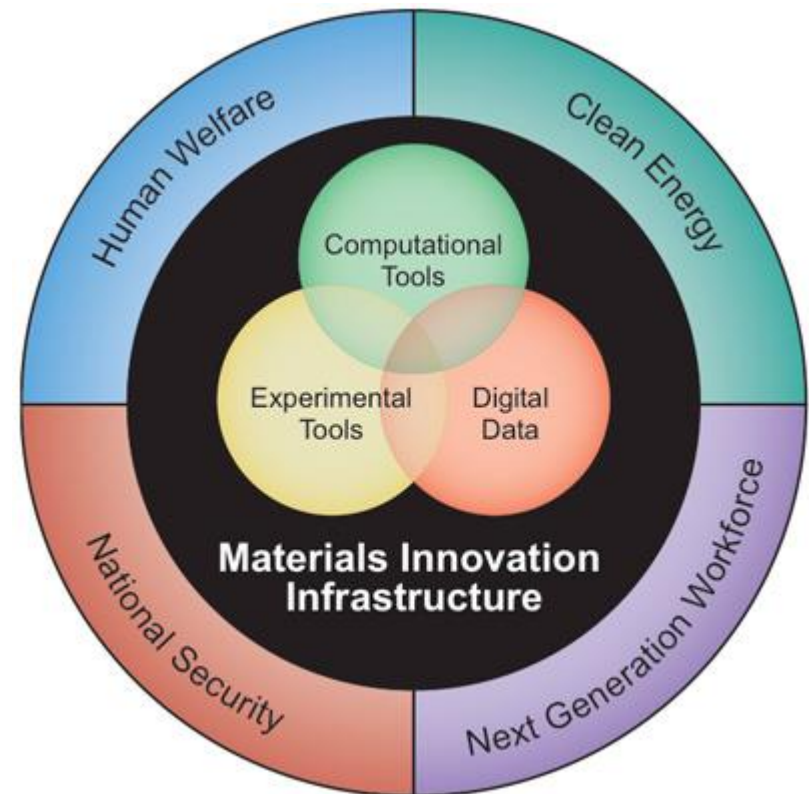
# What is MGI?



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?

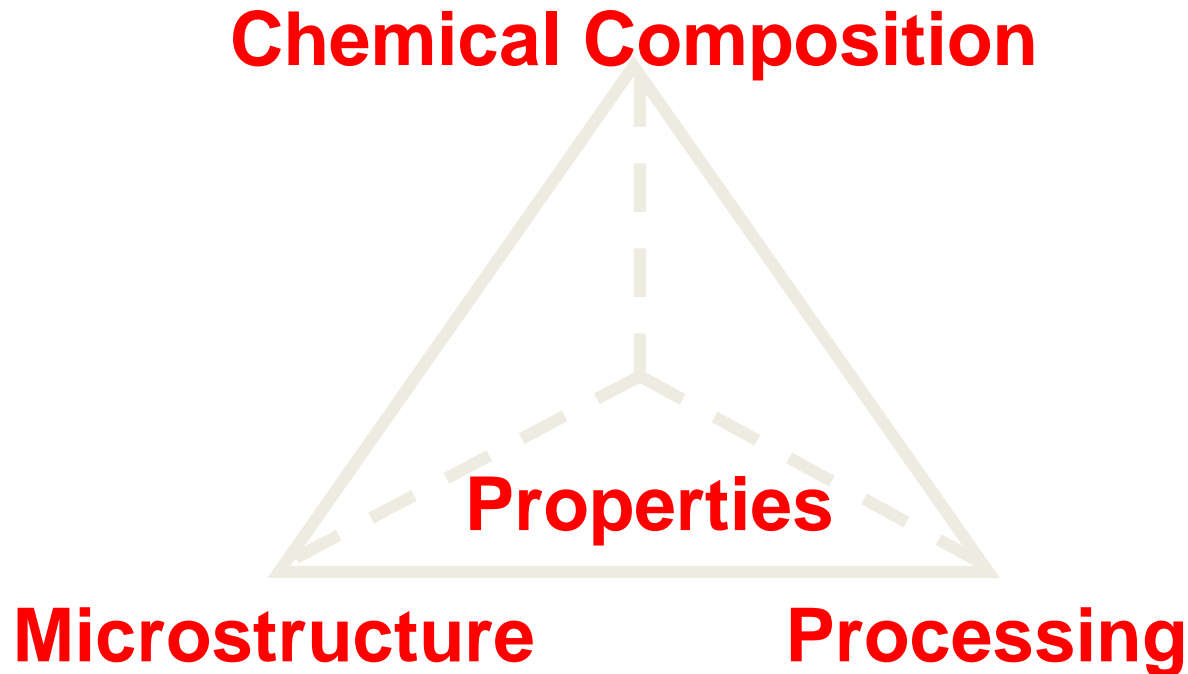
The analogy of a materials genome to a human genome implies that something of the nature of the material is encoded in the the chemical composition of a material and that we should be able to read this.

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

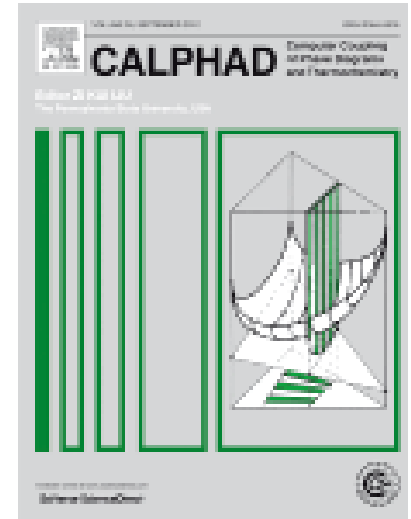


Heat treating can best be defined as “the controlled application of time, temperature and atmosphere to produce a predictable change in the internal structure (i.e. the microstructure) of a material.” Dan Herring, 100th Column of the “Heat Treat Doctor” published in Industrial Heating magazine

# What is CALPHAD? (1)



## CALculation of PHAse Diagrams

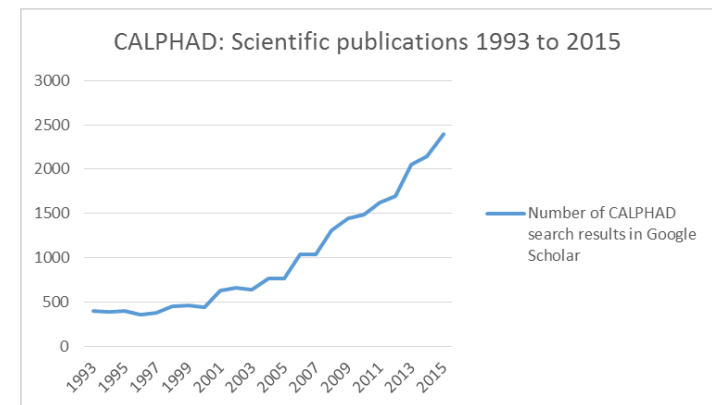


CALPHAD based tools lie at the nexus of composition, temperature, property relationships.

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.

A journal published by Elsevier Ltd.

An international community, and conference held each year with 150-300 active participants from around the world.





# What is CALPHAD (2)

## Thermochemical measurements:

- Enthalpy
- Entropy
- Heat capacity
- Activity

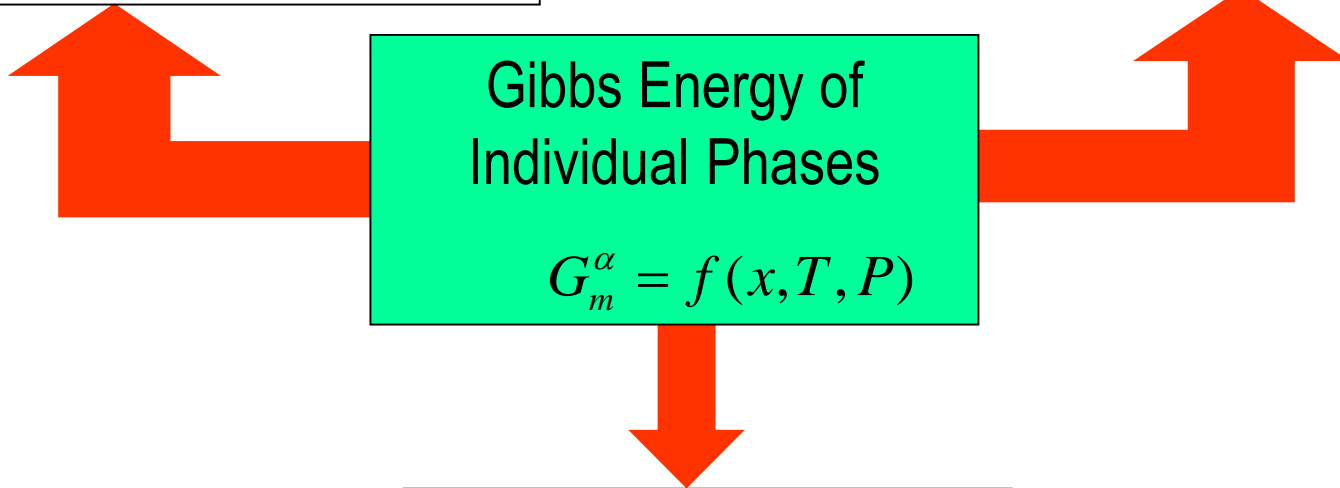
## Phase equilibria:

- Liquidus
- Solidus
- Phase boundary

Gibbs Energy of  
Individual Phases

$$G_m^\alpha = f(x, T, P)$$

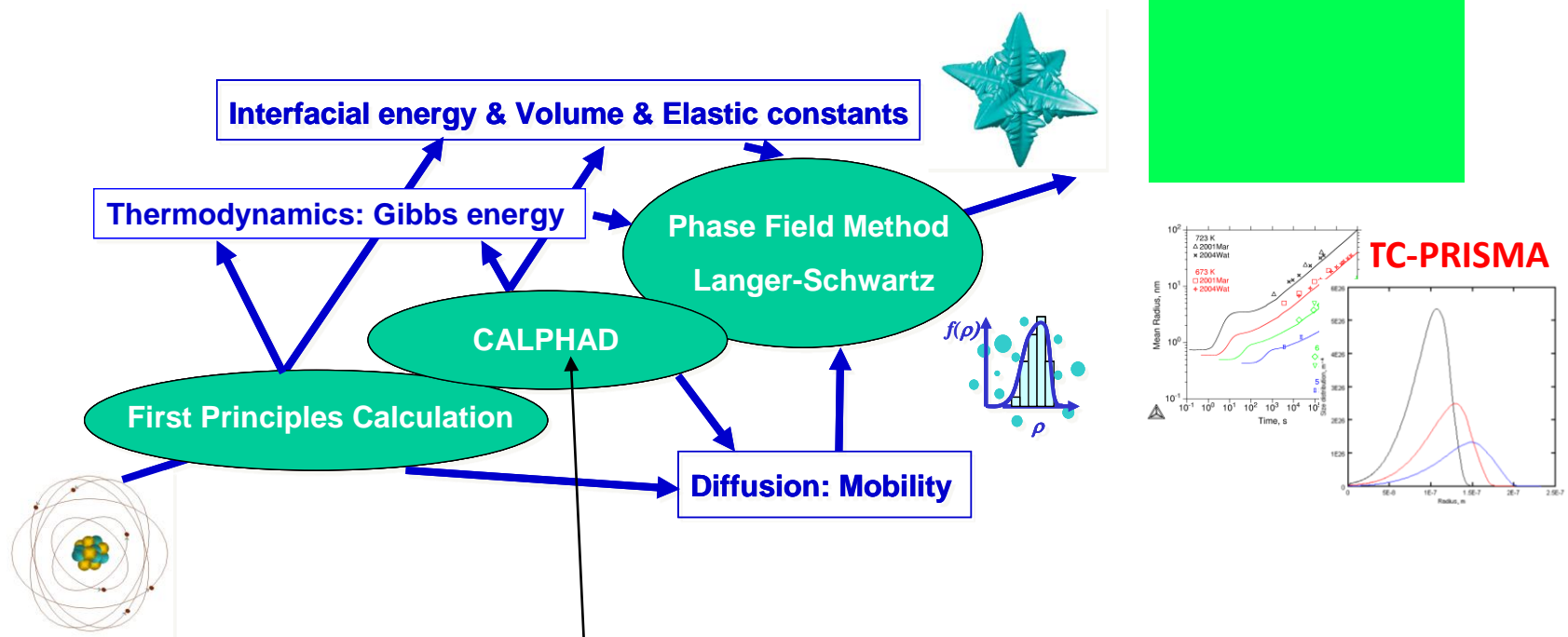
Applications



# CALPHAD – an important bridge to multicomponent prediction

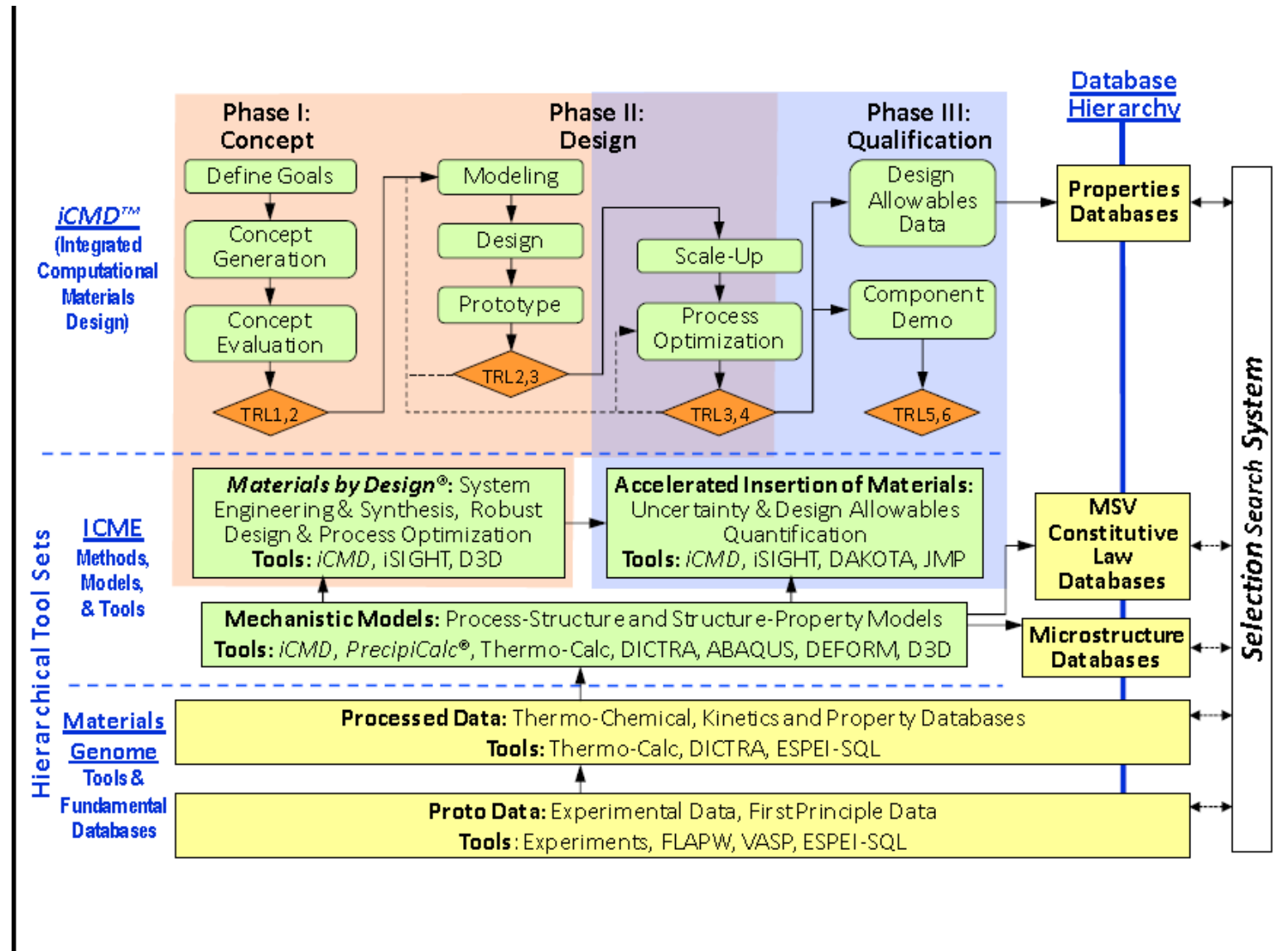
Towards prediction of microstructure evolution and material properties

## *Bridging Atoms and Microstructure*



*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



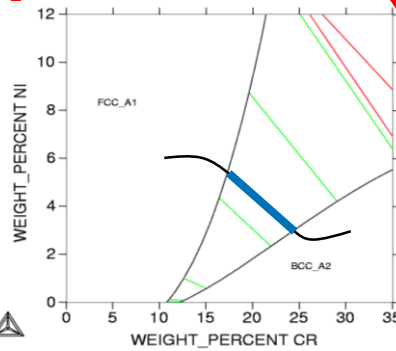
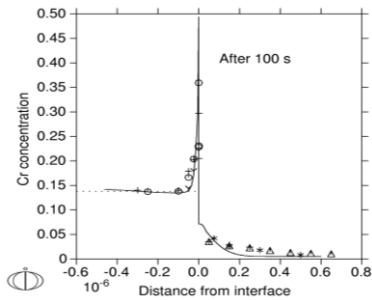
Slide courtesy of Prof. G. Olson, Northwestern University, QuesTek Innovations LLC

# A suite of CALPHAD based software tools

## THERMO-CALC

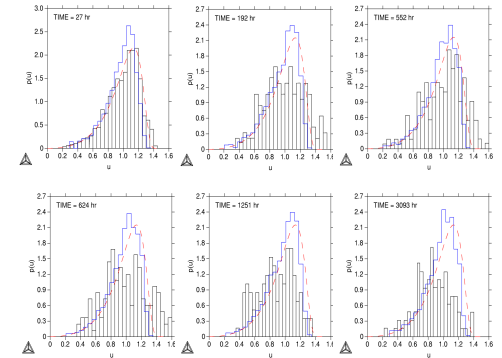
*Driving forces*

### DICTRA

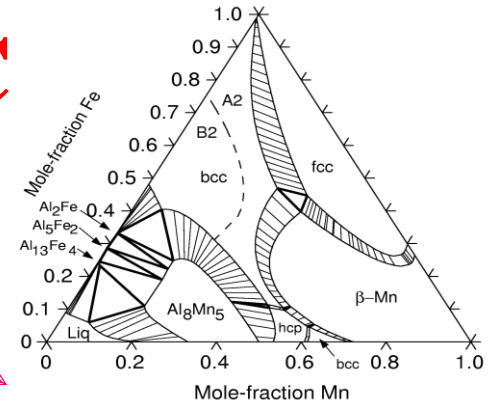


*Interfacial energies*

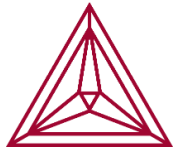
### TC-PRISMA



*Diffusivities*



# Software + Databases - Putting it together



## Thermo-Calc

Minimization of the total Gibbs free energy under given conditions.

$$G = \sum_{\phi} N^{\phi} G_m^{\phi}(T, P, x_i^{\phi})$$

$$\frac{\partial G}{\partial x_i^{\phi}} = 0$$



## DICTRA

1-D diffusion simulation - Numerically solve diffusion equations

**Solve Diffusion**

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial z} (\mathbf{J}) \quad \text{where} \quad \mathbf{J} = -\mathbf{D} \frac{\partial c}{\partial z}$$



## TC-PRISMA

Mean field precipitation simulation – using LS (Langer-Schwartz) and KWN (Kampmann and Wagner Numerical) Approach

Continuity equation

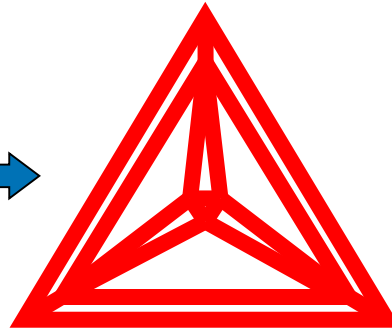
$$\frac{\partial f(r,t)}{\partial t} = -\frac{\partial}{\partial r} [\nu(r)f(r,t)] + j(r,t)$$

$$C_0^{\alpha} = C^{\alpha} + (C^{\beta} - C^{\alpha}) \int_0^{\infty} \frac{4\pi}{3} f(r,t) r^3 dr$$

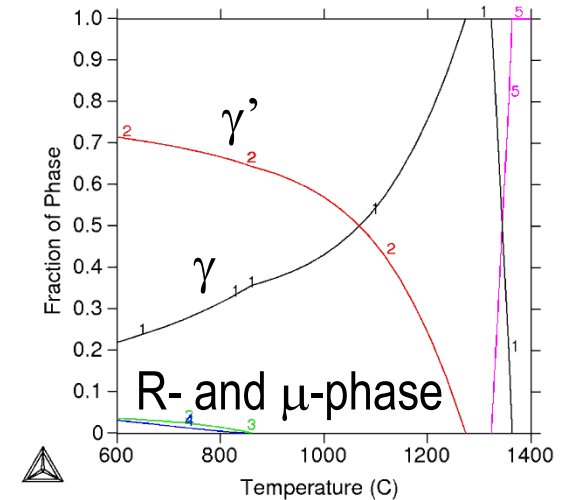
Mass balance

# Importance of databases

Thermodynamic  
Database



Thermo-Calc



Description of Gibbs  
free energy for the  
individual phases

$$G_m^\phi(T, P, x_i^\phi)$$

Minimization of the total  
Gibbs free energy under  
given conditions.

$$G = \sum_{\phi} N^{\phi} G_m^{\phi}(T, P, x_i^{\phi})$$

$$\frac{\partial G}{\partial x_i^{\phi}} = 0$$

Result

A wide range of thermodynamic databases are available for:

- Steels and Fe-alloys
- Nickel-base superalloys
- Aluminium/Titanium/Magnesium-base alloys
- Gases, pure inorganic/organic substances, & general alloys
- Slag, metallic liquids, and molten salts
- Ceramic systems, and hard materials
- Semiconductors, and solder alloys
- Noble metal alloys
- Materials processing, process metallurgical & environmental aspects
- Aqueous solutions, materials corrosion & hydrometallurgical systems
- Minerals, and geochemical/environmental processes
- Nuclear materials, and nuclear fuel/waste processing

# TCNI5 – An example of a multicomponent CALPHAD database

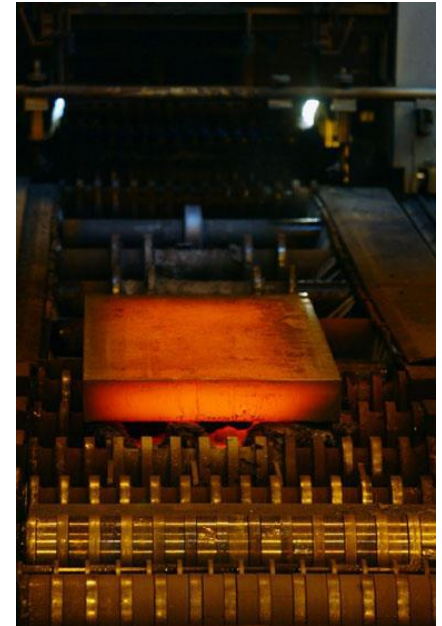
	Al	B	C	Co	Cr	Fe	Hf	Mo	N	Nb	Ni	Pd	Pt	Re	Si	Ta	Ti	V	W
B	x																		
C	x	x																	
Co	x	x	x																
Cr	x	x	x	x															
Fe	x	x	x	x	x														
Hf	x	x	x	x	x	x													
Mo	x	x	x	x	x	x	x												
N	x	x		x	x	x		x											
Nb	x	x	x	x	x	x	x	x	x										
Ni	x	x	x	x	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
- Total number of possible ternaries (1140)
- All Ni containing ternaries plus other ternary systems also assessed to full range of composition (184 / 1140 in total)
- 292 intermetallic and solution phases



# CALPHAD based software: Thermo-Calc (1)

- 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

## Single Pt Eqm

```

Output from POLY-3
Tue Aug 08 2006 11:41:39
Database: TCFE3

Conditions:
T=1000, P=1E5, N=1, W(C)=2E-2, W(CR)=0.1, W(MN)=3E-2, W(NI)=1E-2
DEGREES OF FREEDOM 0

Temperature 1000K (727C, 1340F), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass 5.16905E+01
Total Gibbs energy -4.42393E+04, Enthalpy 2.56582E+04, Volume 5.22429E-06

Component      Moles      W-Fraction    Activity      Potential      Ref.State
C                8.6072E-02  2.0000E-02    8.9724E-02    -2.0046E+04    SER
CR               9.9412E-02  1.0000E-01    4.4290E-04    -6.4206E+04    SER
FE               7.7748E-01  8.4000E-01    6.0347E-03    -4.2489E+04    SER
MN               2.8227E-02  3.0000E-02    4.6517E-05    -8.2943E+04    SER
NI               8.8074E-03  1.0000E-02    3.3158E-05    -8.5758E+04    SER

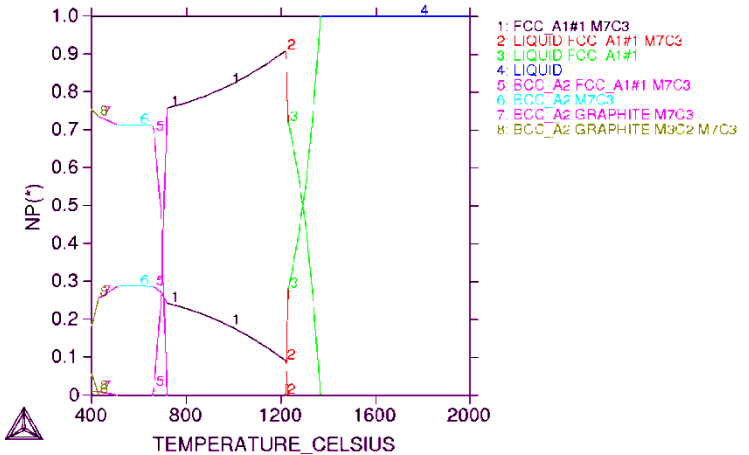
FCC_A1#1        STATUS ENTERED      Driving force 0.0000E+00
Number of moles 7.5868E-01, Mass 4.1735E+01
Mass fractions:
FE 9.44835E-01 CR 1.41596E-02 C 3.93605E-03
MN 2.47653E-02 NI 1.23038E-02

FCC_A1#2        STATUS ENTERED      Driving force 0.0000E+00
Number of moles 0.0000E+00, Mass 0.0000E+00
Mass fractions:
FE 9.44835E-01 CR 1.41596E-02 C 3.93605E-03
MN 2.47653E-02 NI 1.23038E-02

M7C3#1         STATUS ENTERED      Driving force 0.0000E+00
Number of moles 2.4132E-01, Mass 9.9559E+00
Mass fractions:
CR 4.59839E-01 C 8.73393E-02 NI 3.42660E-04
FE 4.00536E-01 MN 5.19435E-02
    
```

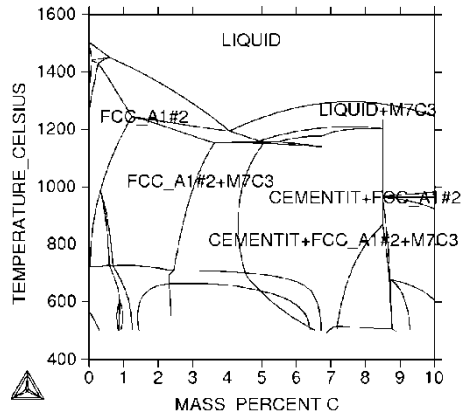
## STEP

THERMO-CALC (2006.08.08:11.43) :  
 DATABASE:TCFE3  
 P=1E5, N=1, W(C)=2E-2, W(CR)=0.1, W(MN)=3E-2, W(NI)=1E-2;



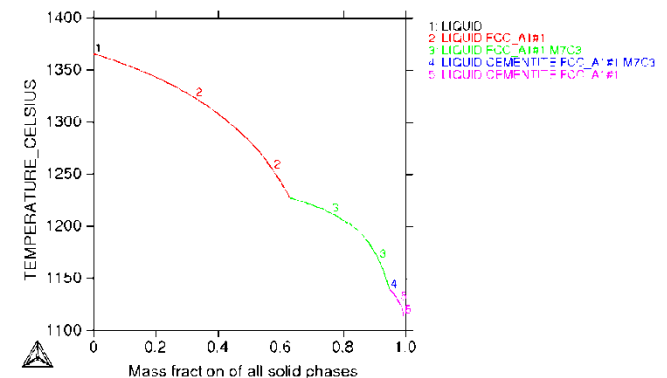
## MAP

THERMO-CALC (2006.08.08:11.46) :  
 DATABASE:TCFE3  
 P=1E5, N=1, W(CR)=0.1, W(MN)=3E-2, W(NI)=1E-2;



## SCHEIL

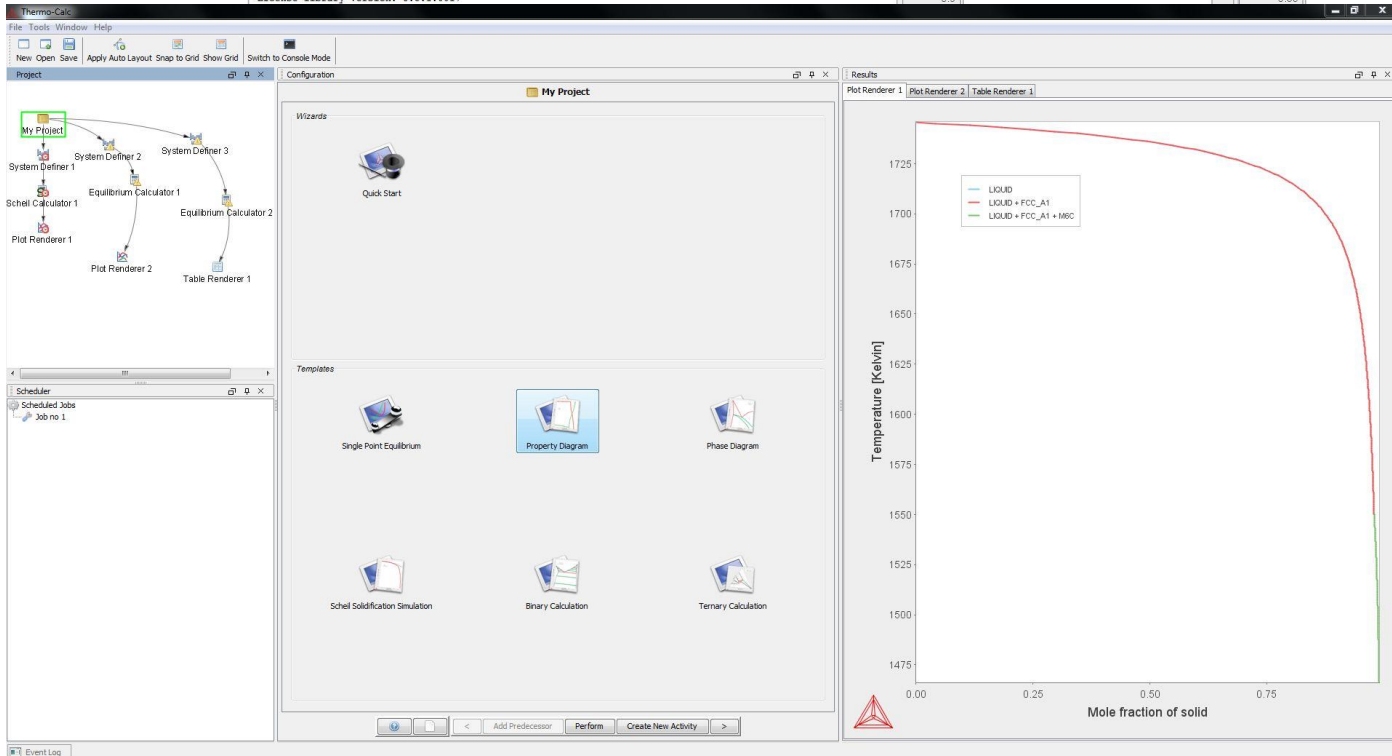
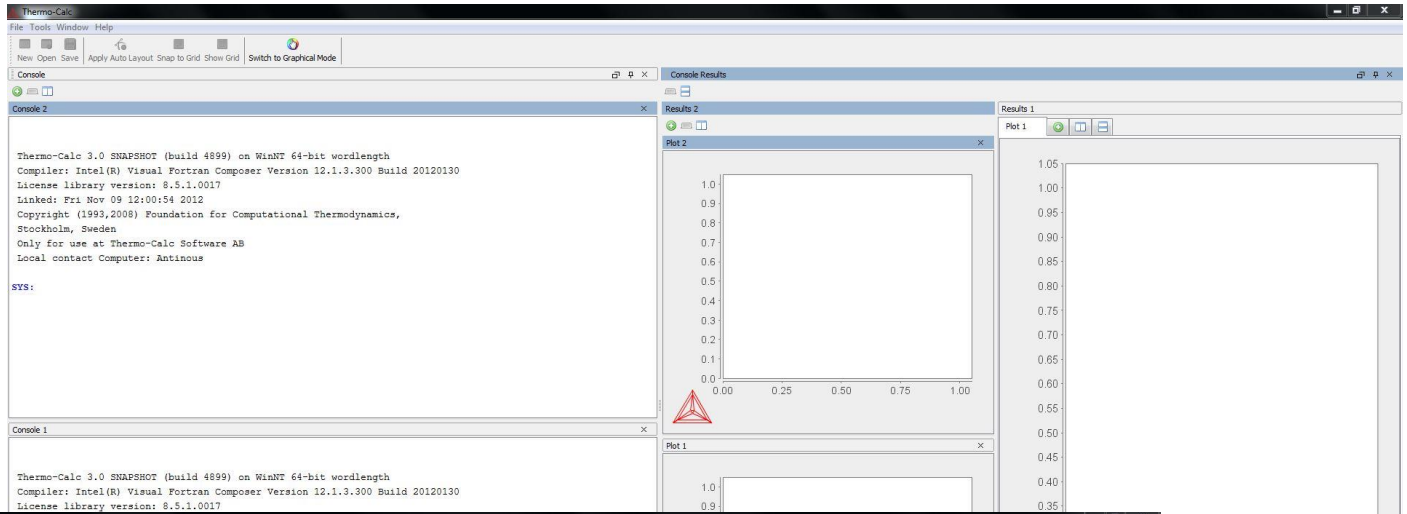
THERMO-CALC (2006.08.08:11.47) :  
 DATABASE:TCFE3



# Overview of Thermo-Calc 2019a



## Console Mode



## Graphical Mode

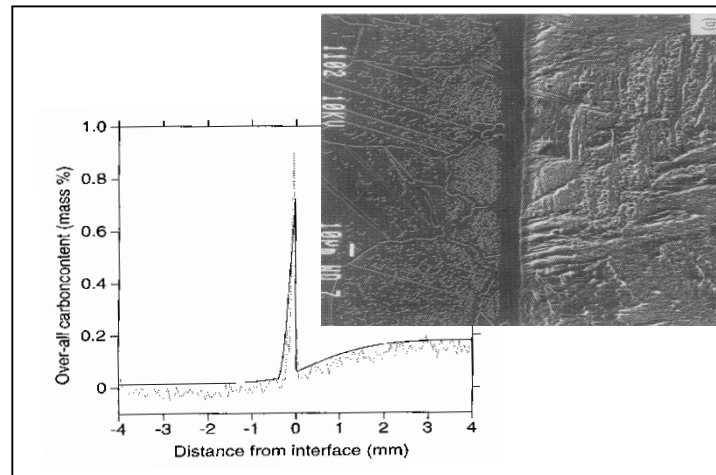
# Early example using thermodynamic calcs in alloy design

- The first systematic use 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*

- A general software package for simulation of **D**iffusion **C**ontrolled **T**Ransformations in multi component alloys.
- The result of more than 20 years and 60 man-years R&D at:
  - Royal Institute of Technology (KTH) in Stockholm, Sweden
  - Max-Planck Institute für Eisenforschung in Düsseldorf, Germany

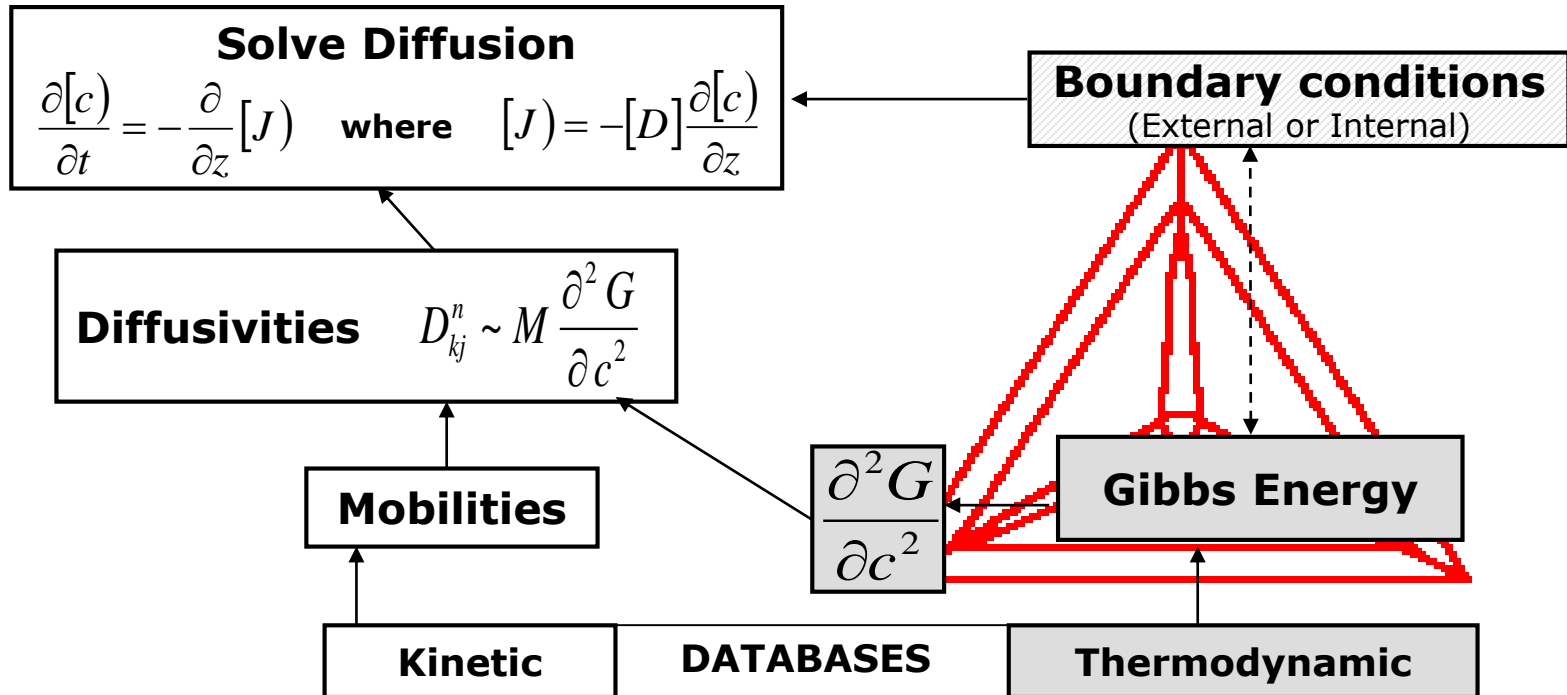
## ***Example: Interdiffusion in compound***



***Emphasis has been placed on linking fundamental methods to critically assessed thermodynamic and kinetic data, allowing simulations and predictions to be performed with realistic conditions on alloys of practical importance.***

# CALPHAD based software: DICTRA (2)

*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.

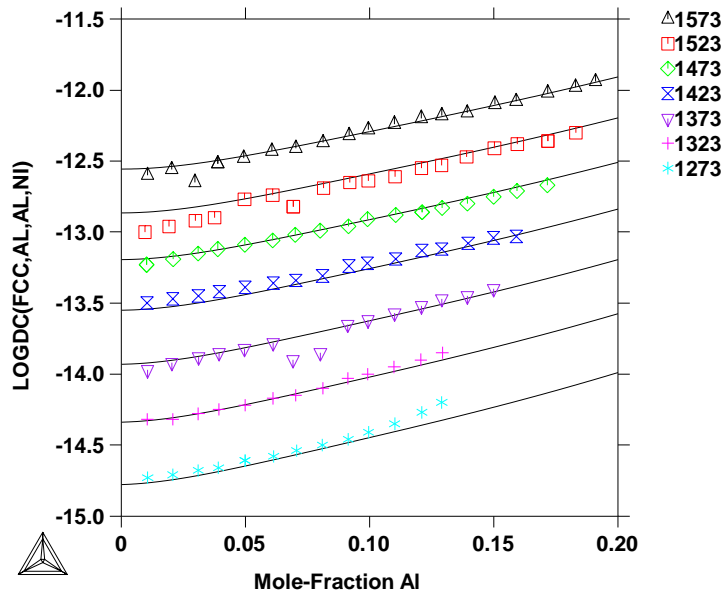
# Diffusion rates are needed

- Modelling must apply in multicomponent systems because the real alloys are multicomponent. Many diffusion coefficients!
- Various type of coupling effects may make it more complicated than Fick's law.
- Details of geometry not of primary importance.
- An approach in the Calphad spirit was suggested for information on diffusion kinetics (Andersson-Ågren 1992)
  - Allowed systematic representation of the kinetic behaviour of multicomponent alloy systems.
- DICTRA was developed in the 1990s for numerical solution of multicomponent diffusion problems in simple geometries.

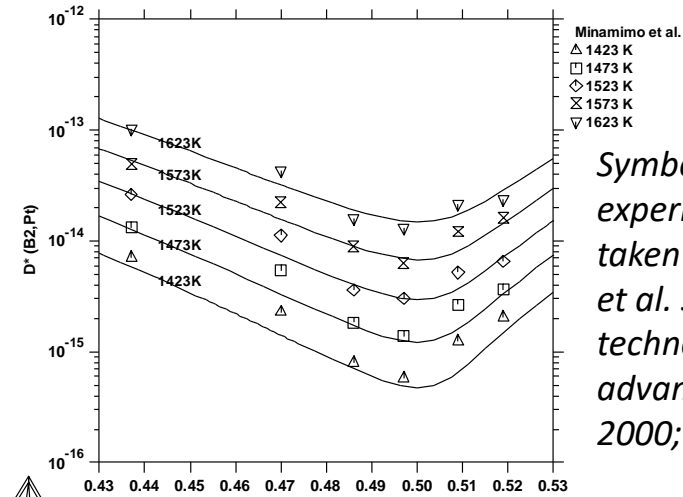
*Slide courtesy of Prof. J. Ågren, KTH*

## Mobility databases are currently available for:

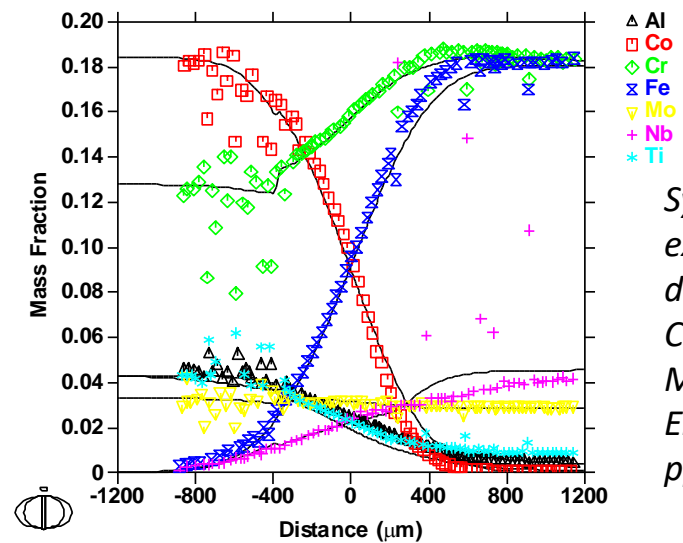
- Steels and Fe-alloys
- Nickel-base superalloys
- Aluminium alloys
- Titanium alloys
- Copper and Magnesium alloys
- HEAs and Solders



Symbols are experimental data taken from Yamamoto et al, *Trans. Jpn. Inst. Met.* **21**(1980), p. 601.



Symbols are experimental data taken from Minamino et al. *Science and technology of advanced materials* 2000;1:237-249.

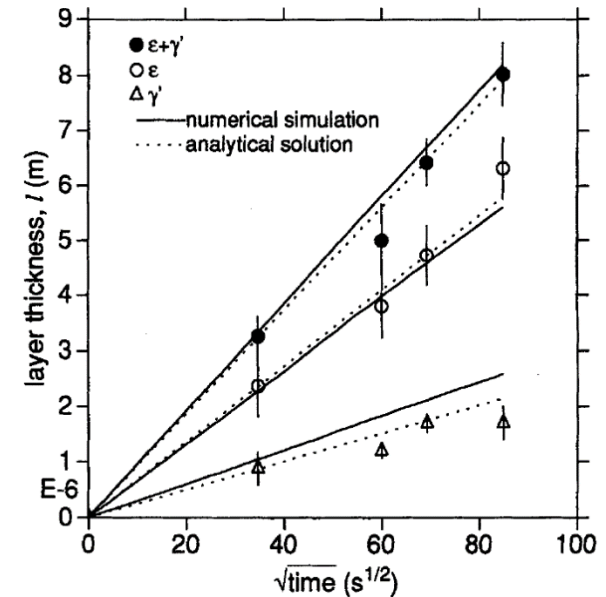
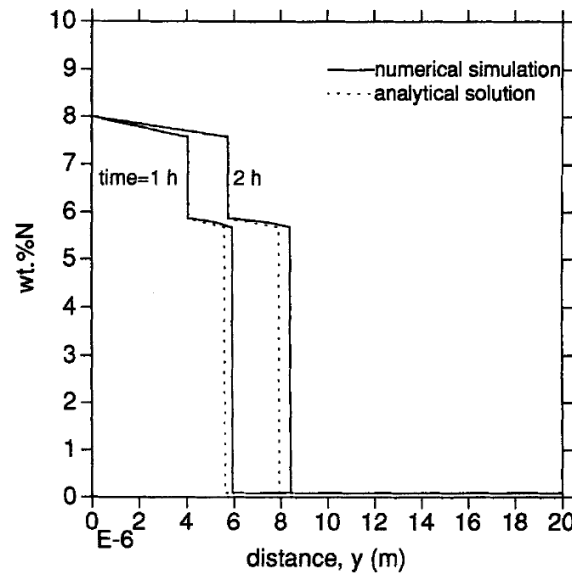
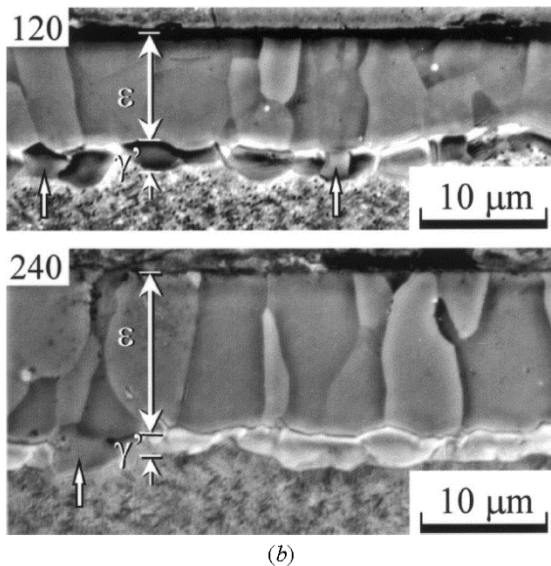


Symbols are experimental data taken from Campbell et al, *Materials Sci & Eng A* **407**(2005), pp. 135-146.



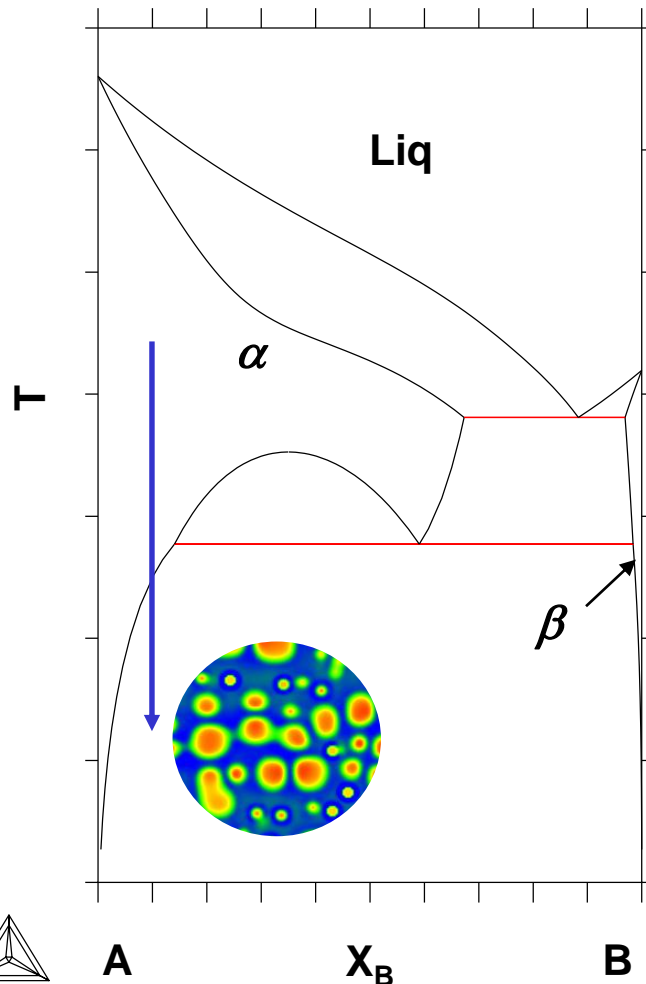
# Example of thermodynamics + diffusion - Nitriding

- Nitride formation at steel surface during nitriding of steel: (Du et al. 1996, 1998)
- A surface modification process with many advantages. How thick are the surface layers?



# CALPHAD based software: TC-PRISMA (1)

- Simulate concurrent nucleation, growth and coarsening of second phases in multicomponent systems.
- Integrated directly with Thermo-Calc and DICTRA.



T  
C  
P  
R  
I  
S  
M  
A

- Particle Size Distribution
- Number Density
- Average Particle Radius
- Volume Fraction
- TTT/CCT
- Average Compositions
- Interface Compositions
- Nucleation Rate
- Critical Radius



## Classic Nucleation Theory

Grain size, dislocation density, etc

$$J(t) = J_s \exp\left(-\frac{\tau}{t}\right)$$

$$J_s = Z\beta^* N \exp\left(\frac{-\Delta G^*}{kT}\right)$$

Interfacial energy Volume

$$Z = \left\{ \frac{-1}{2\pi kT} \left( \frac{\partial^2 \Delta G_n}{\partial n^2} \right)_{n^*} \right\}^{1/2}$$

$$\Delta G^* = \frac{16\pi\sigma^3 V_m^2}{3\Delta G_m^2}$$

$$\beta^* = \frac{4\pi r^{*2}}{a^4} \left[ \sum_{i=1}^n \frac{(X_i^{\beta/\alpha} - X_i^{\alpha/\beta})^2}{X_i^{\alpha/\beta} D_i} \right]^{-1}$$

$$\tau = \frac{1}{2Z^2 \beta^*}$$

# The need for interfacial energies

The length scale is typically determined by a combination of thermodynamic driving forces, interfacial energy, diffusion and the dynamic nature of the process.

Modelling and databases for interfacial energy needed.

In the simplest case interfacial energy is just a number (which may be difficult to determine experimentally but could be obtained from e.g. coarsening studies). Because of uncertainty could be treated as a calibration factor.

# TC-PRISMA Examples: Ni-based superalloy (1)

Booth-Morrison et al. Acta Mater. 56(2008) 3422-3438

Sudbrack et al. Acta Mater. 56(2008)448-463

Sudbrack et al. Acta Mater. 54(2006)3199-3210

Ni-9.8Al-8.3Cr

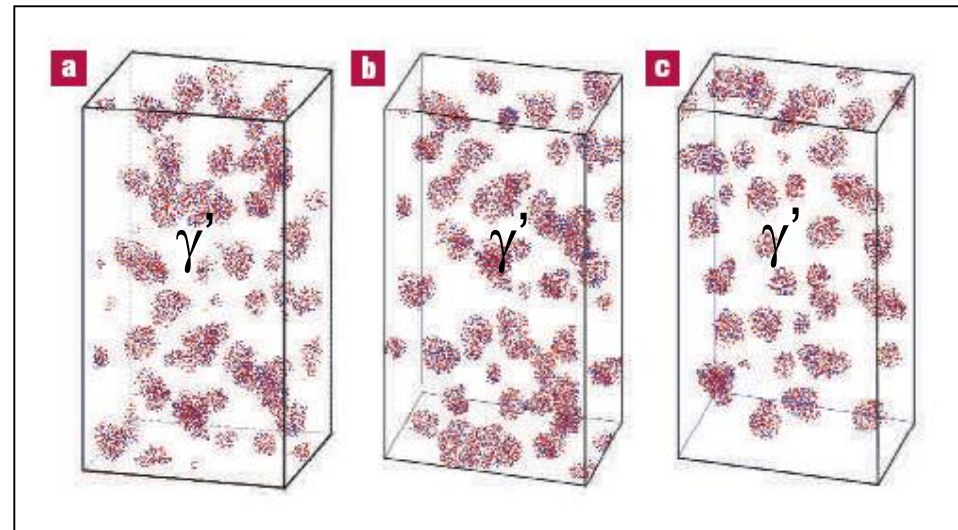
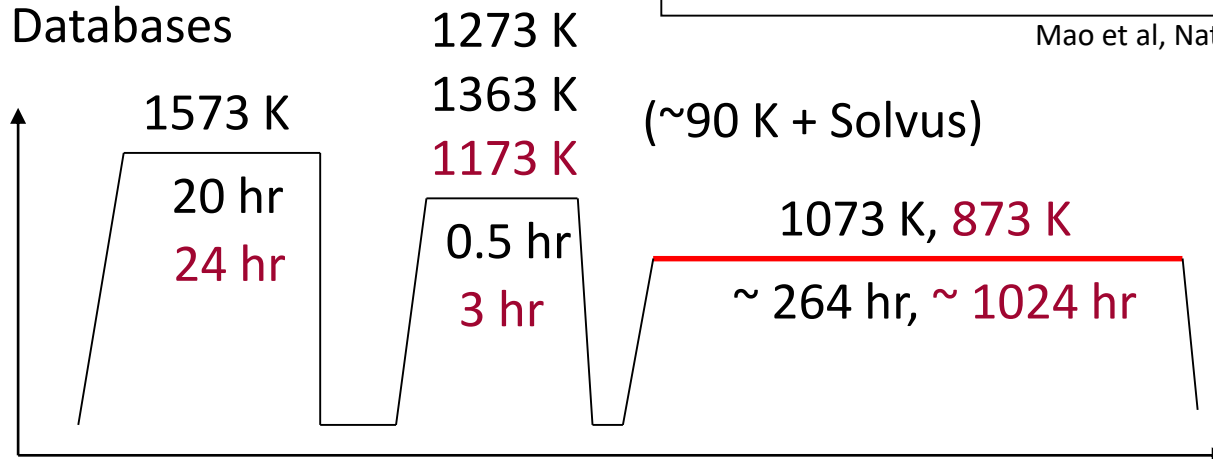
Ni-9.7Al-8.5Cr-2W

Ni-7.5Al-8.5Cr

Ni-5.2Al-14.2Cr

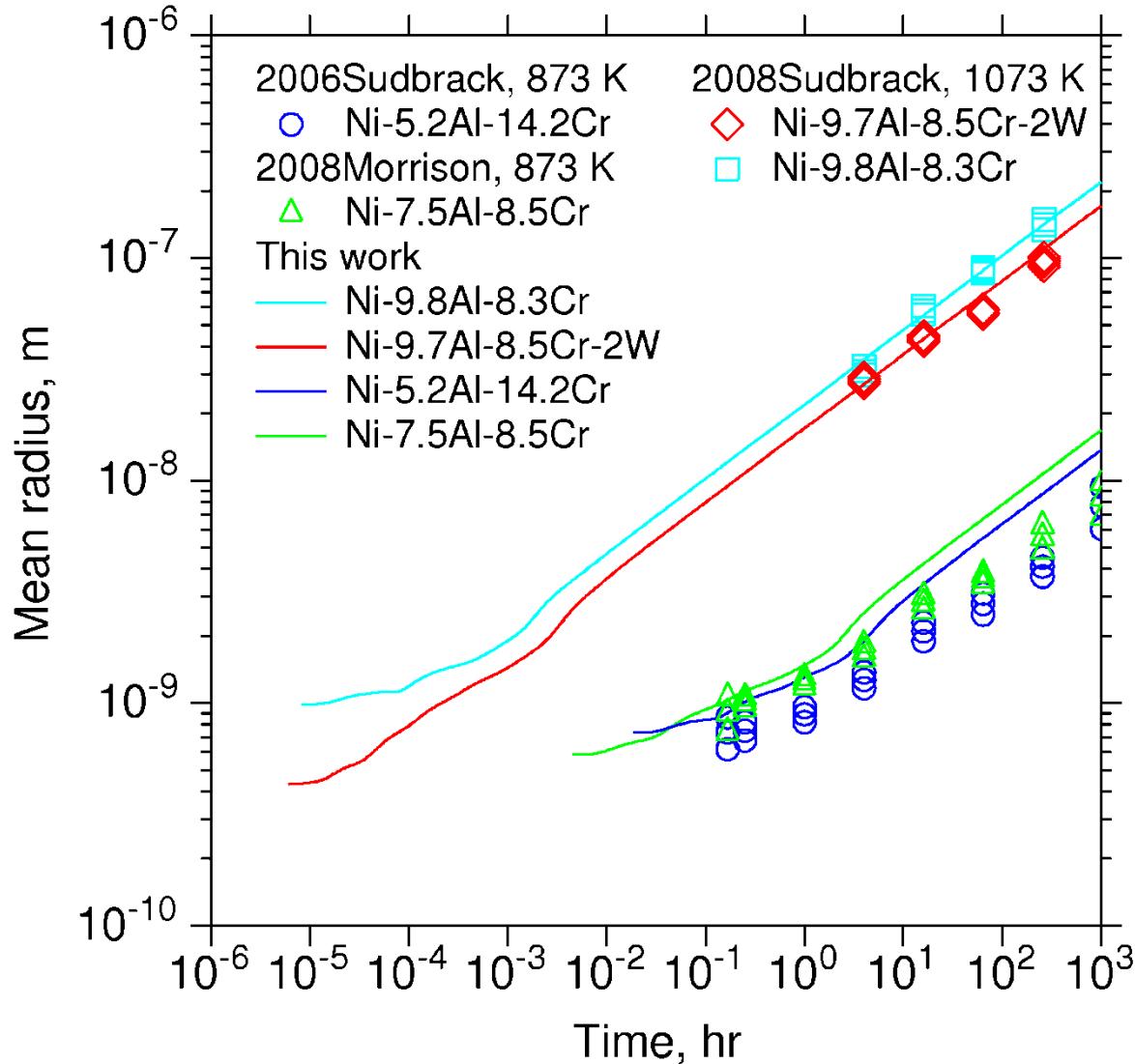
$s = 0.023 \text{ J/m}^2$

Thermo-Calc and Dictra  
Databases

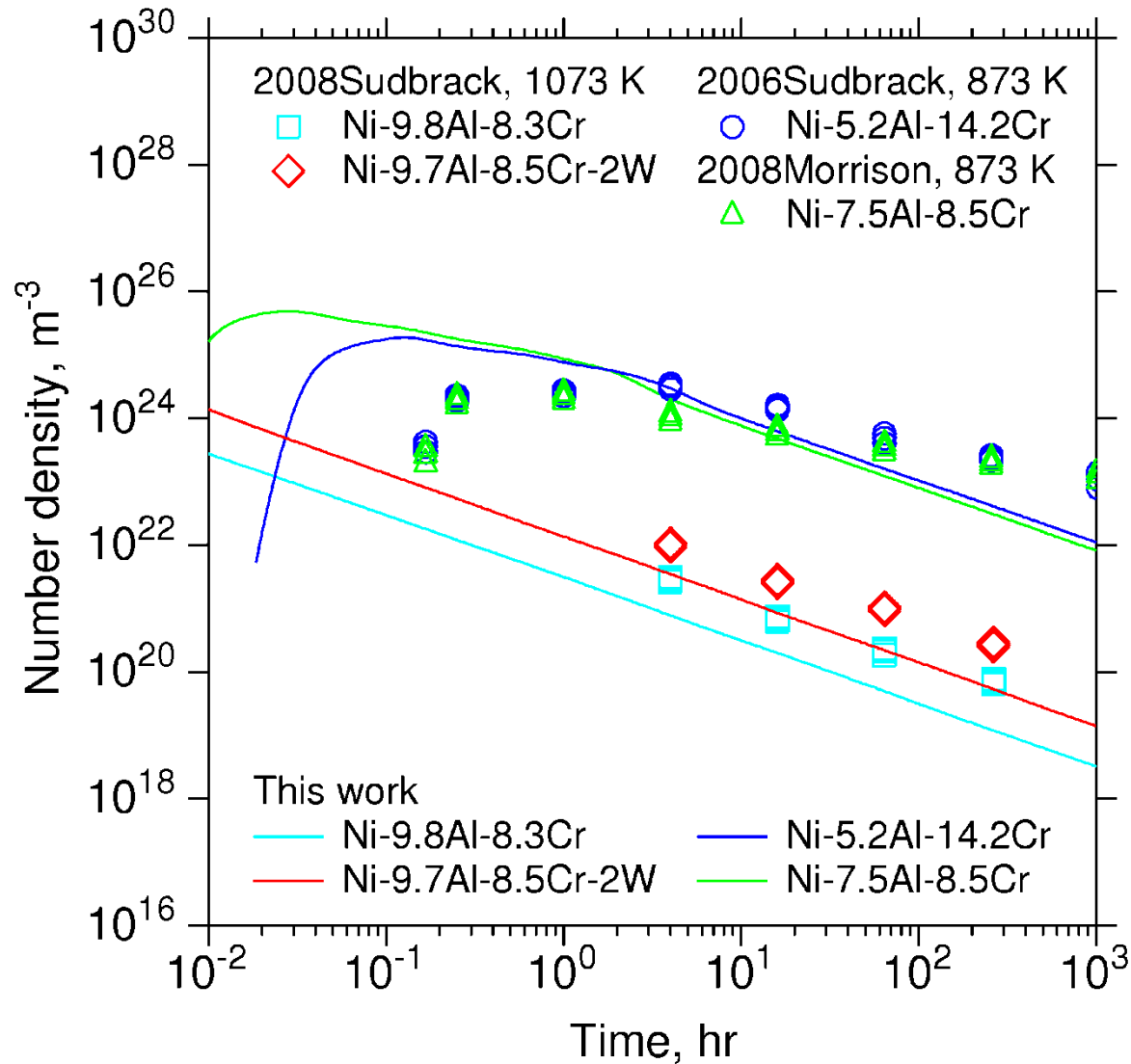


Mao et al, Nature materials, 6(2007)210-216

# TC-PRISMA Examples: Ni-based superalloy (2) – Mean radius

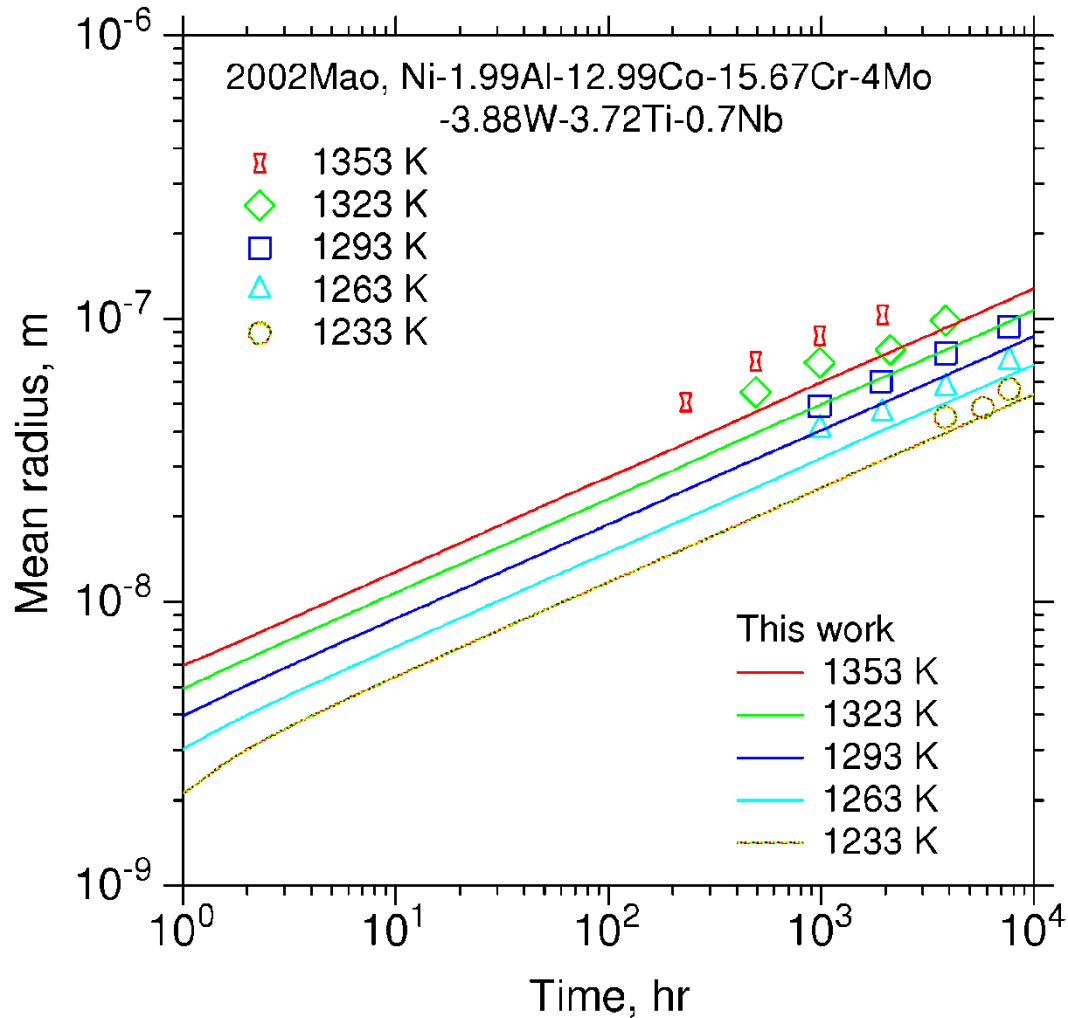


# TC-PRISMA Examples: Ni-based superalloy (3) – Number density



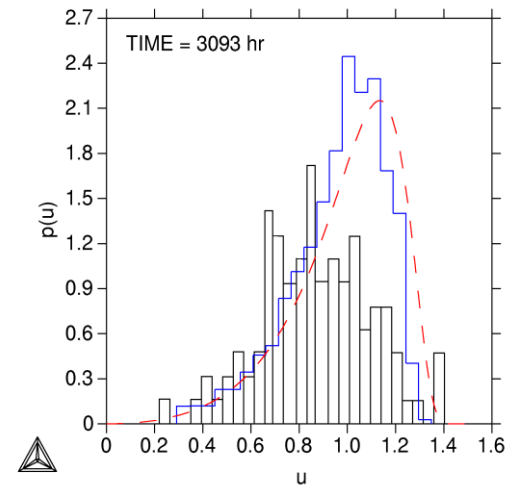
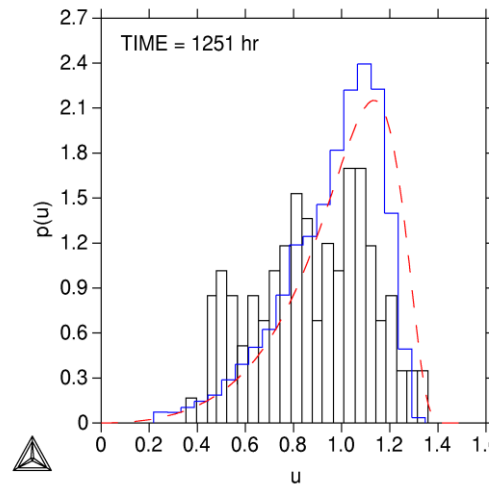
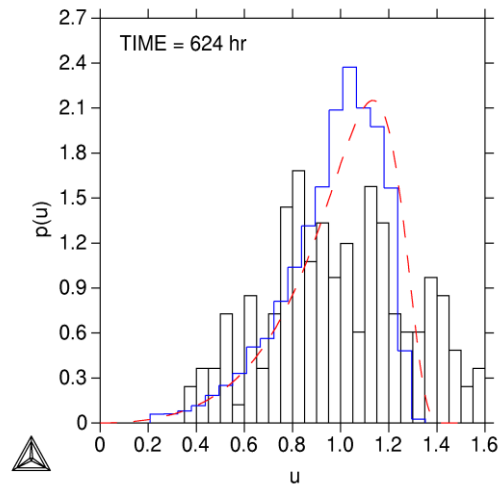
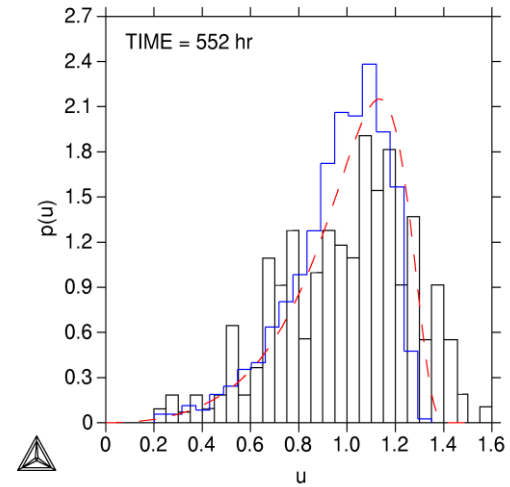
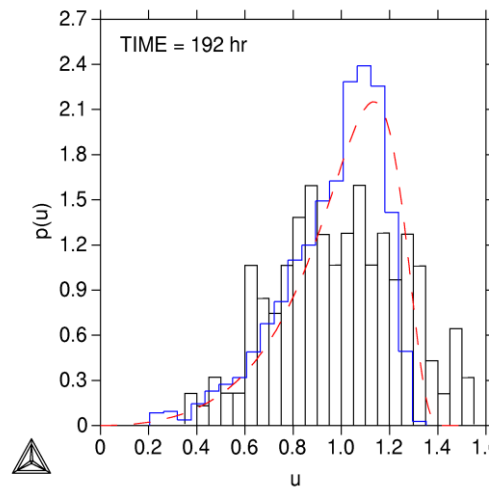
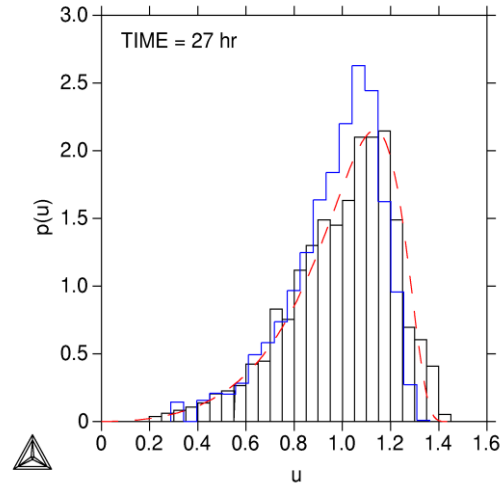
# TC-PRISMA Examples: Ni-based superalloy (4) – Rene88DT

Change only system and use same set of physical parameters





# TC-PRISMA Examples: Particle size distribution



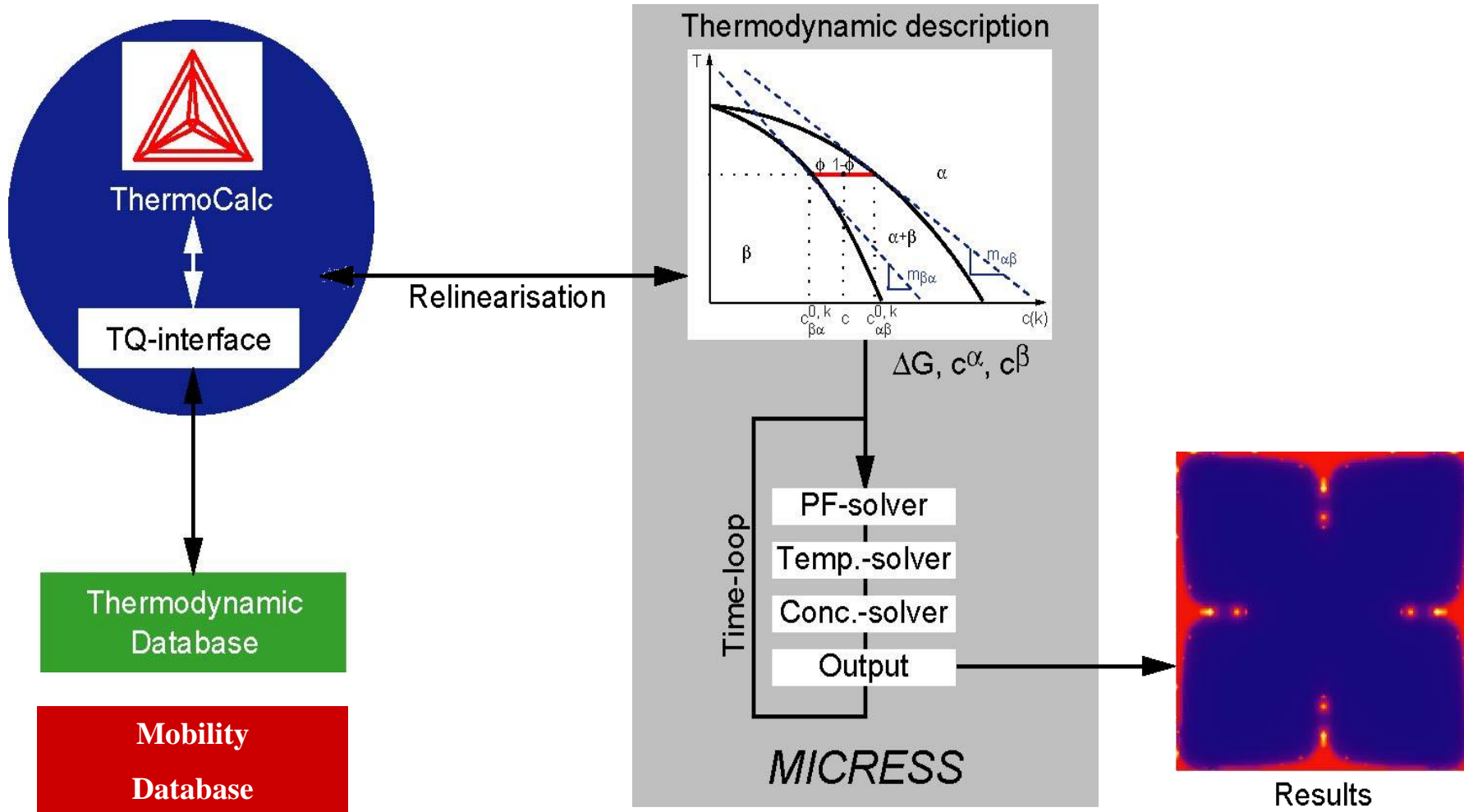
# CALPHAD based software: Phase field (1)

- 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)
  - ....

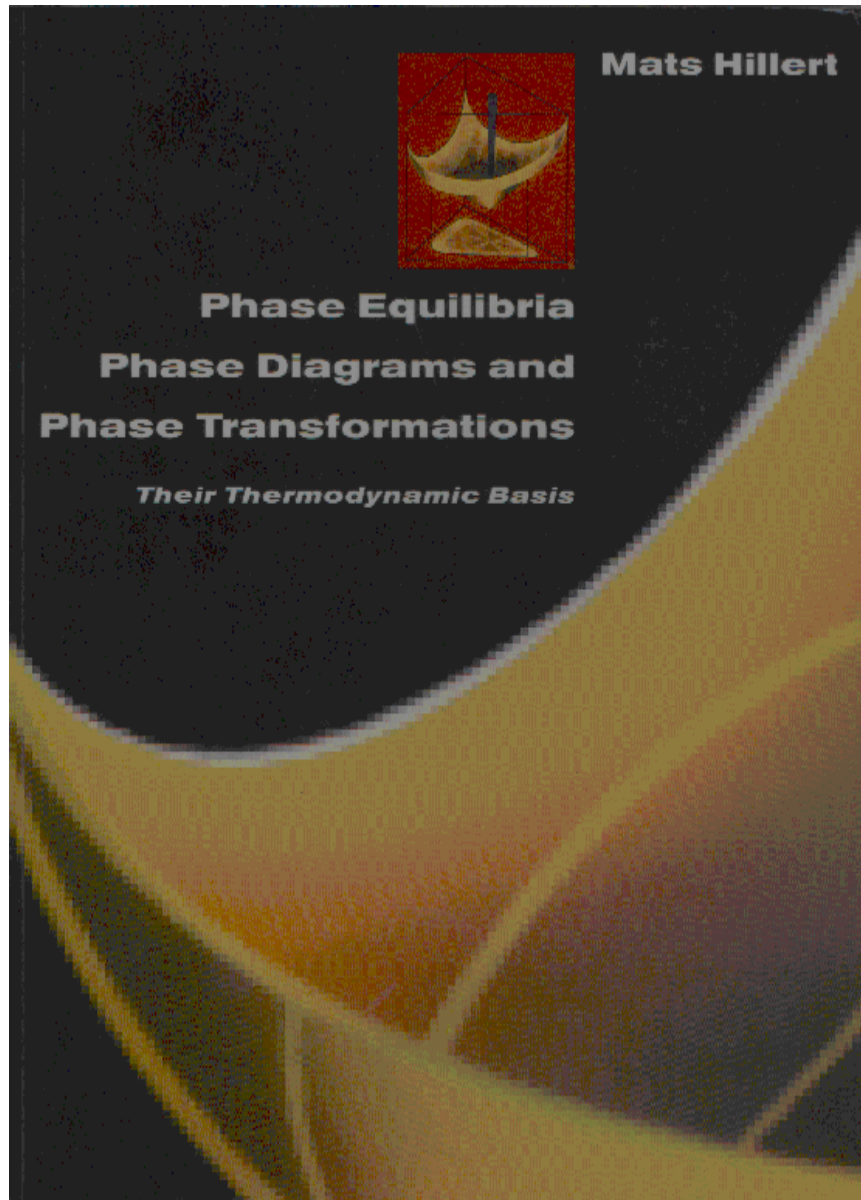
*Slide courtesy of Prof. J. Ågren, KTH*

# CALPHAD based software: Phase field (2)

Slide courtesy of Dr. Georg J. Schmitz, ACCESS

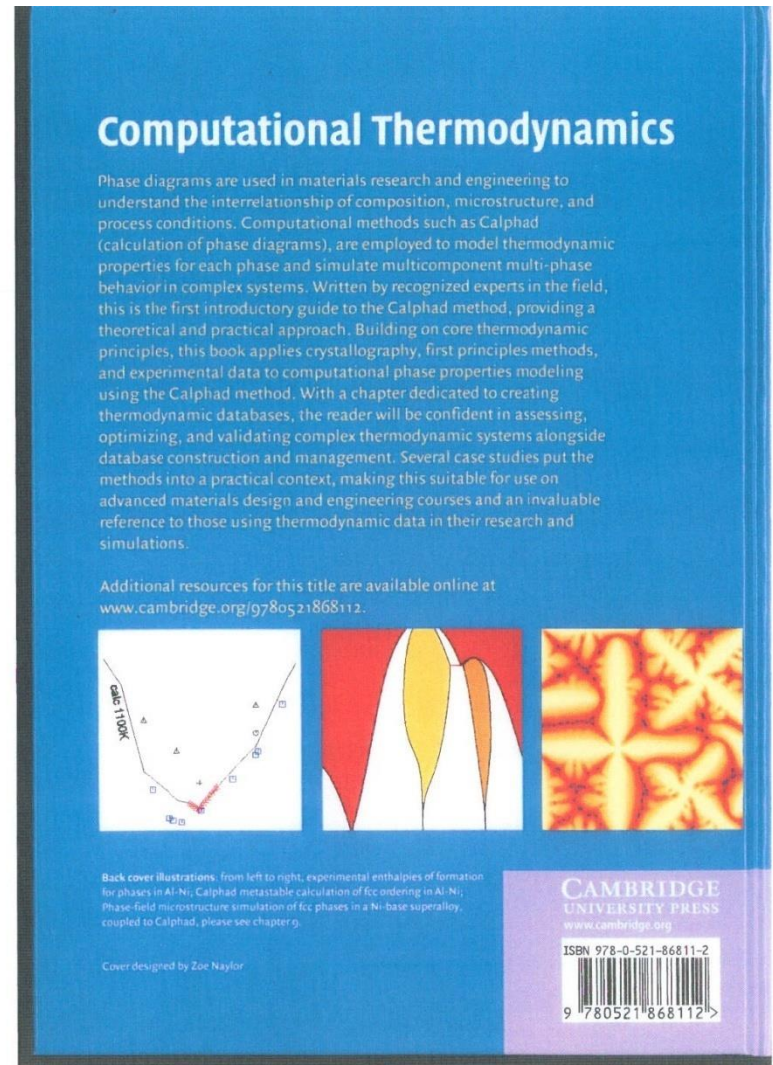
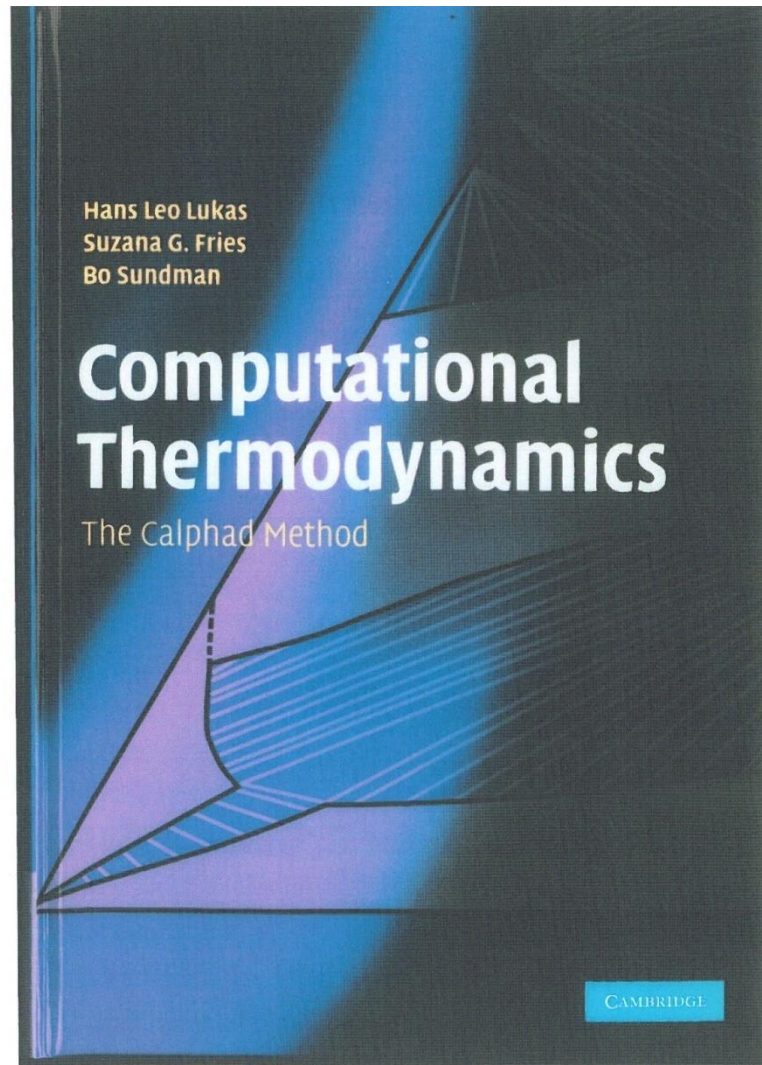


# The underlying principles Of CALPHAD and Thermo-Calc



ISBN 978-0-521-85351-4





ISBN 978-0-521-86811

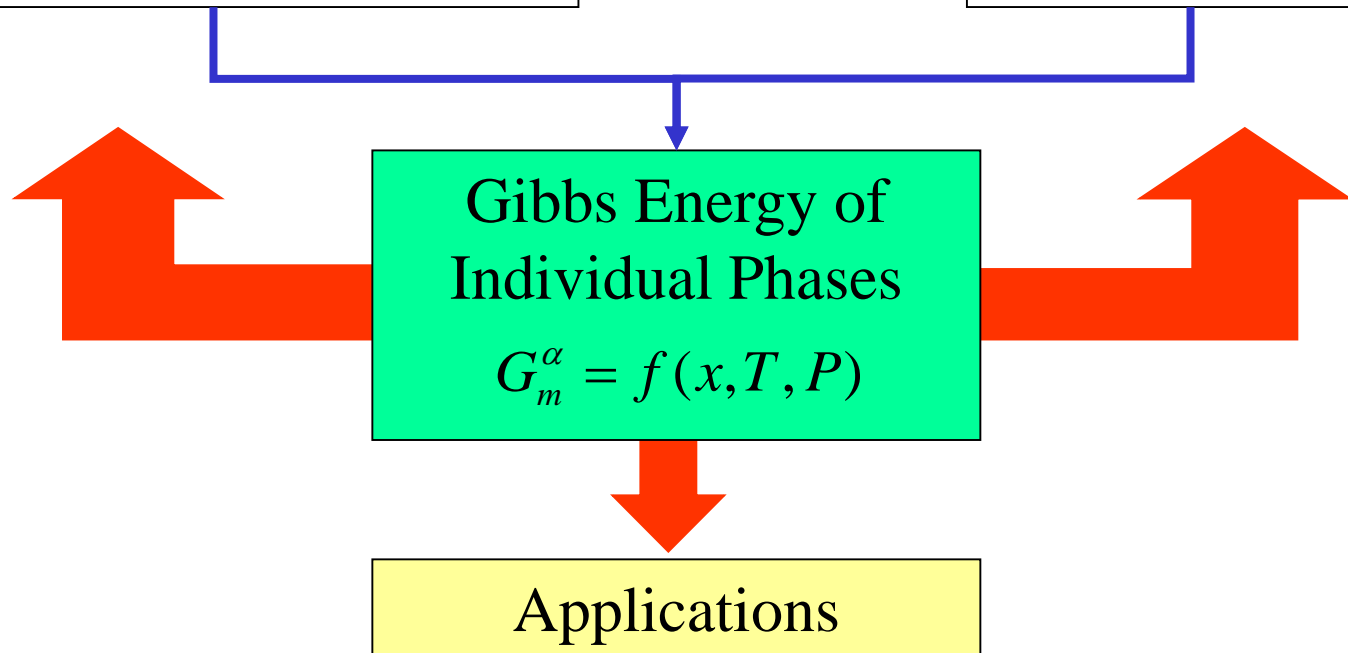
## Thermodynamic Databases (*The CALPHAD approach*)

### Thermochemical measurements:

- Enthalpy
- Entropy
- Heat capacity
- Activity

### Phase equilibria:

- Liquidus
- Solidus
- Phase boundary



# Gibbs Energy

## Gibbs Free Energy $\Leftrightarrow$ Phase Diagram

$$G = \sum_{\phi} N^{\phi} G_m^{\phi}(T, P, x_i^{\phi})$$

$$\frac{\partial G}{\partial x_i^{\phi}} = 0$$

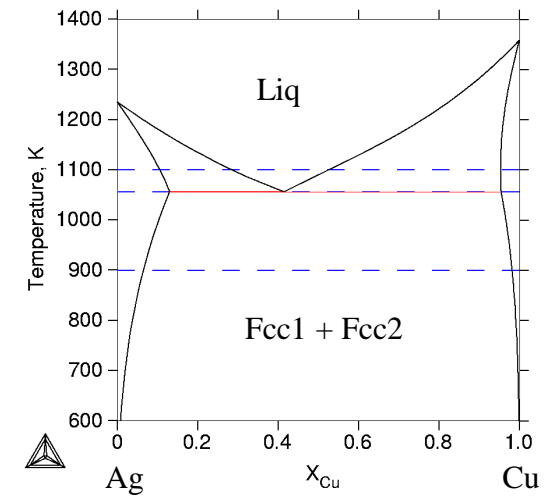
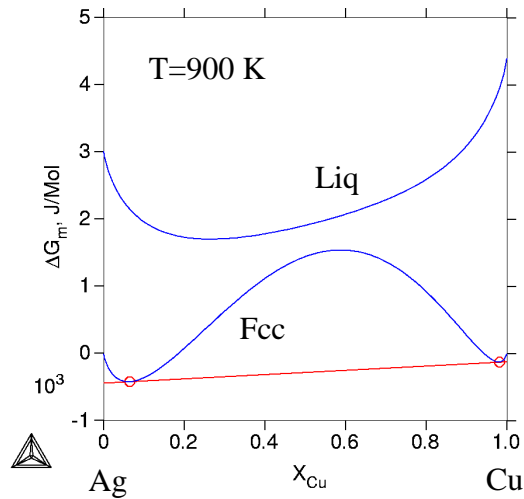
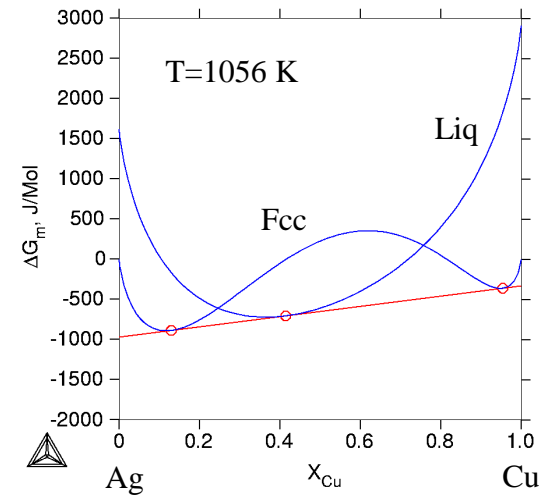
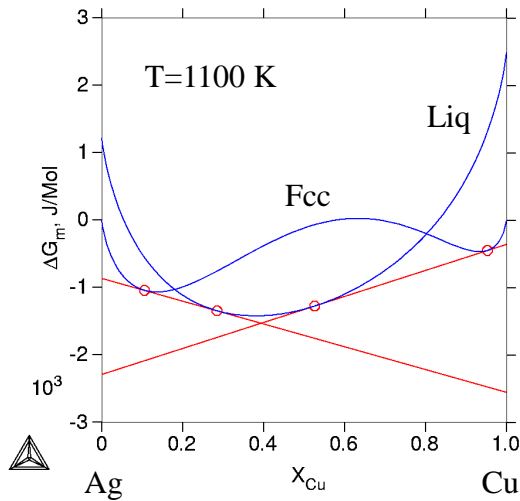
### Why Gibbs free energy?

Most experiments under constant T and P

Gibbs energy is the state function minimized under constant T and P at the state of equilibrium.



# Underlying thermodynamics



## Reference state

Pure elements/substances

$$G_m - H_m^{SER} = a + bT + cT \ln(T) + \sum d_i T^i$$

- Gibbs energy relative to a standard element reference state (SER), i.e. the enthalpy of the element in its stable state at 298.15K and 0.1MPa. GHSEFE means the Gibbs energy of FE under SER state.
- Entropy at 0K = 0 (+TS(0))
- Needed because there is no absolute value of the enthalpy of a system and one must select some reference state.
- For a reference state, one can change its phase structure, temperature, and pressure.

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

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

reference surface                      configurational contribution                      excess term                      physical contribution

- Ideal solution model
- Regular solution model
- Real solution

# Binary - Ideal Solution Model

For a A-B binary solution phase: (A,B)

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

$$G_m^0 = x_A G_A^o + x_B G_B^o$$

$$\Delta G_m^{ideal} = RT \left( x_A \ln x_A + x_B \ln x_B \right)$$

# Binary - Regular solution model

$$G_m = G_m^0 + \Delta G_m^{ideal} + \Delta G_m^{xs}$$

$$G_m^0 = x_A G_A^o + x_B G_B^o$$

$$\Delta G_m^{ideal} = RT(x_A \ln x_A + x_B \ln x_B)$$

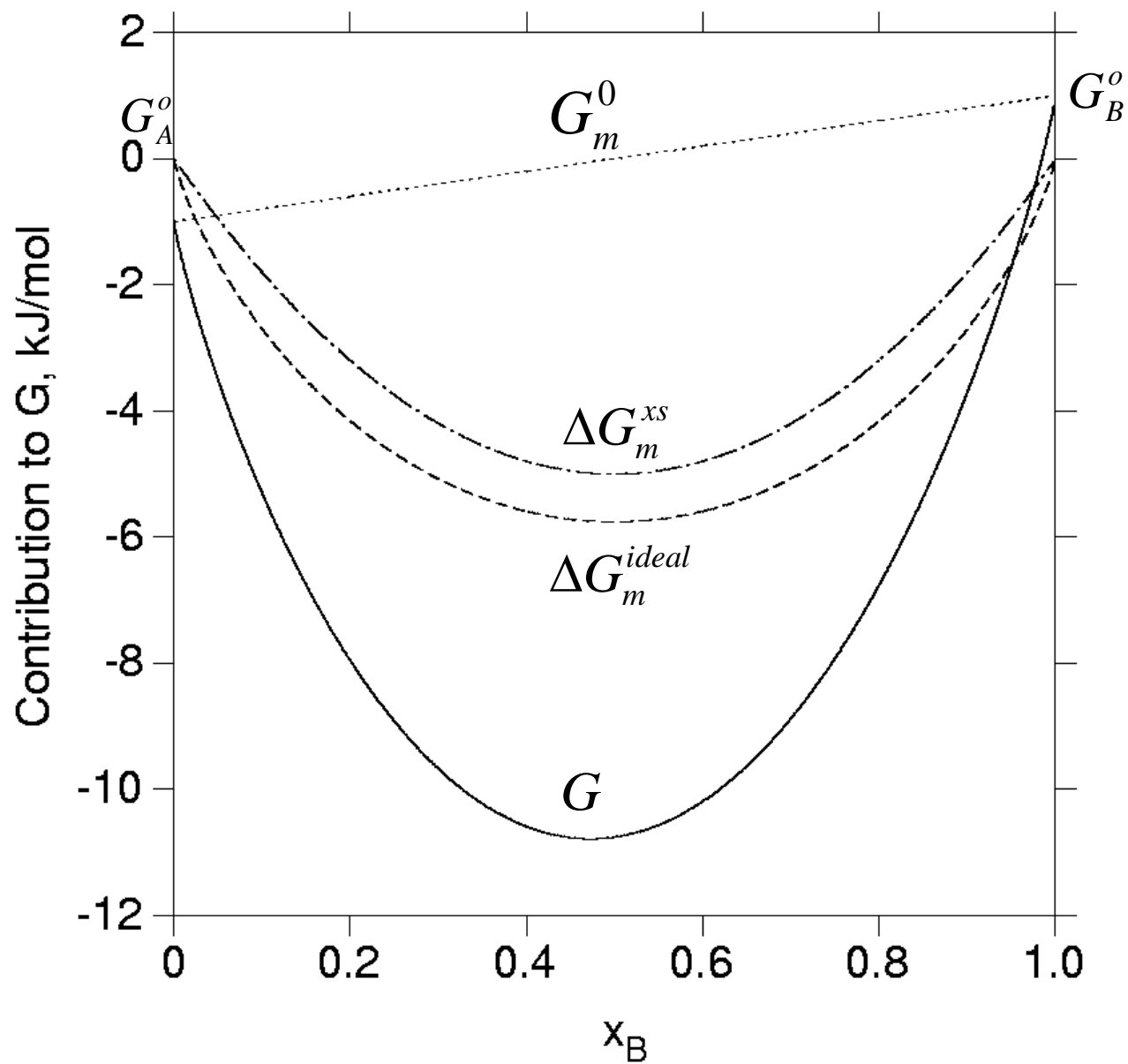
$$\Delta G_m^{xs} = x_A x_B {}^0L_{A,B}$$

$${}^0L_{A,B} = a + bT$$

$$\Delta S_m^{xs} = -x_A x_B b$$

$$\Delta H_m^{xs} = x_A x_B a$$

$$\Delta C_P^{xs} = 0$$



# Binary - Real solutions

$$G_m = G_m^0 + \Delta G_m^{ideal} + \Delta G_m^{xs}$$

$$G_m^0 = x_A G_A^o + x_B G_B^o$$

$$\Delta G_m^{ideal} = RT(x_A \ln x_A + x_B \ln x_B)$$

## Redlich-Kister Expansion

$$\begin{aligned} \Delta G_m^{xs} &= x_A x_B \sum_{k=0}^{\infty} L_{A,B} (x_A - x_B)^k \\ &= x_A x_B \left( {}^0L_{A,B} + {}^1L_{A,B} (x_A - x_B) + {}^2L_{A,B} (x_A - x_B)^2 \dots \right) \end{aligned}$$

# Ternary solutions

$$G_m = G_m^0 + \Delta G_m^{ideal} + \Delta G_m^{xs}$$

$$G_m^0 = x_A G_A^o + x_B G_B^o + x_C G_C^o$$

$$\Delta G_m^{ideal} = RT(x_A \ln x_A + x_B \ln x_B + x_C \ln x_C)$$

$$\Delta G_m^{xs} = \sum_i \sum_{j>i} x_i x_j I_{ij} + \sum_i \sum_{j>i} \sum_{k>j} x_i x_j x_k I_{ijk} + \dots$$

From  
Binary

From  
Ternary



# Thermodynamic models

Thermodynamic models handle EOS & all kinds of thermodynamic properties for various systems. Some of the available models are:

- Component-Energy Model (*interaction on up to ten sublattices*):
  - Redlich-Kister polynomials (Muggianu or Kohler extrapolation)
  - Stoichiometric constraints
  - Interstitial solution
  - Chemical ordering
  - Ionic constituents
- Two-Sublattice Ionic Liquid Model
- Associated Model
- Quasi-chemical Model
- Kapoor-Frohberg Cell Model
- Inden Model for magnetic ordering
- CVM (Cluster Variation Methods) for chemical ordering
- Birch-Murnaghan Model (pressure-dependency) for minerals/alloys
- SUPERFLUID Model for C-H-O-S-N-Ar fluid & gaseous mixtures
- DHLL, SIT, HKF and PITZ Models for aqueous solutions
- Flory-Huggins Model for polymers

# Binary Example of Compound Energy Formalism

$$G_m^{hcp} = x_{Co} {}^0G_{Co}^{nhcp} + x_{Ni} {}^0G_{Ni}^{nhcp} + RT(x_{Co} \ln x_{Co} + x_{Ni} \ln x_{Ni}) \\ + {}^{ex}G_m^{nhcp} + {}^{mag}G_m^{hcp},$$

where

$${}^0G_{elem}^{ph} = a + bT + cT \ln T + dT^{-1} + eT^2 + fT^{-2} + \dots$$

$${}^{ex}G_m^{nhcp} = x_{Co} x_{Ni} \sum_{i=0}^j (x_{Co} - x_{Ni})^i {}^iL_{Co,Ni}^{hcp}$$

$${}^iL_{Co,Ni}^{hcp} = A + BT$$

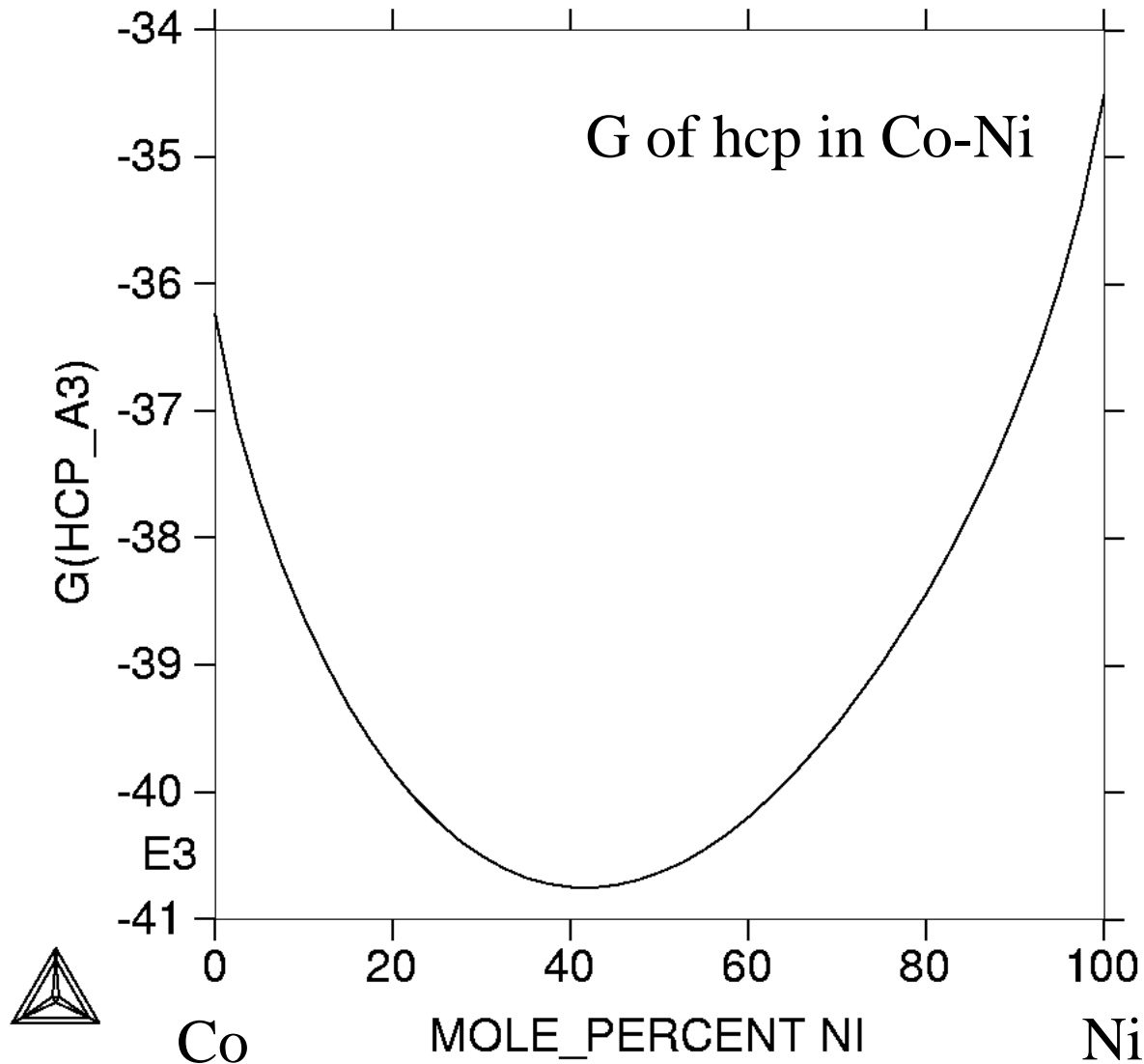
$${}^{mag}G_m^{hcp} = \text{an expression of similar form as } G_m^{hcp}$$

# Simple Binary Example of CEF

```
PARAMETER G (HCP_A3,CO:VA;0) 298.15 +GHSERCO;,,N !
PARAMETER G (HCP_A3,NI:VA;0) 298.15 +GHCPNI;,,N !
FUNCTION GHSERCO 298.15 +310.241+133.36601*T
-25.0861*T*LN(T)-.002654739*T**2-1.7348E-07*T**3
+72527*T**(-1) 1768.0 Y -17197.666+253.28374*T
-40.5*T*LN(T)+9.3488E+30*T**(-9);,, N !
FUNCTION GHSEJNI 298.15 -5179.159+117.854*T
-22.096*T*LN(T)-.0048407*T**2;
1728.0 Y -27840.655+279.135*T-43.1*T*LN(T)
+1.12754E+31*T**(-9);,, N !
PARAMETER L (HCP_A3,CO,NI:VA;0) 298.15 -1620-.385*T;,,N !
PARAMETER TC (HCP_A3,CO:VA;0) 298.15 +1396;,,N !
PARAMETER BMAGN (HCP_A3,CO:VA;0) 298.15 1.35;,,N !
PARAMETER TC (HCP_A3,NI:VA;0) 298.15 633;,,N !
PARAMETER BMAGN (HCP_A3,NI:VA;0) 298.15 .52;,,N !
PARAMETER TC (HCP_A3,CO,NI:VA;0) 298.15 411;,,N !
PARAMETER TC (HCP_A3,CO,NI:VA;1) 298.15 -99;,,N!
PARAMETER BMAGN (HCP_A3,CO,NI:VA;0) 298.15 1.046;,,N !
PARAMETER BMAGN (HCP_A3,CO,NI:VA;1) 298.15 .165;,,N !
```

# Simple Binary Example of CEF

THERMO-CALC (2001.11.21:14.59) :

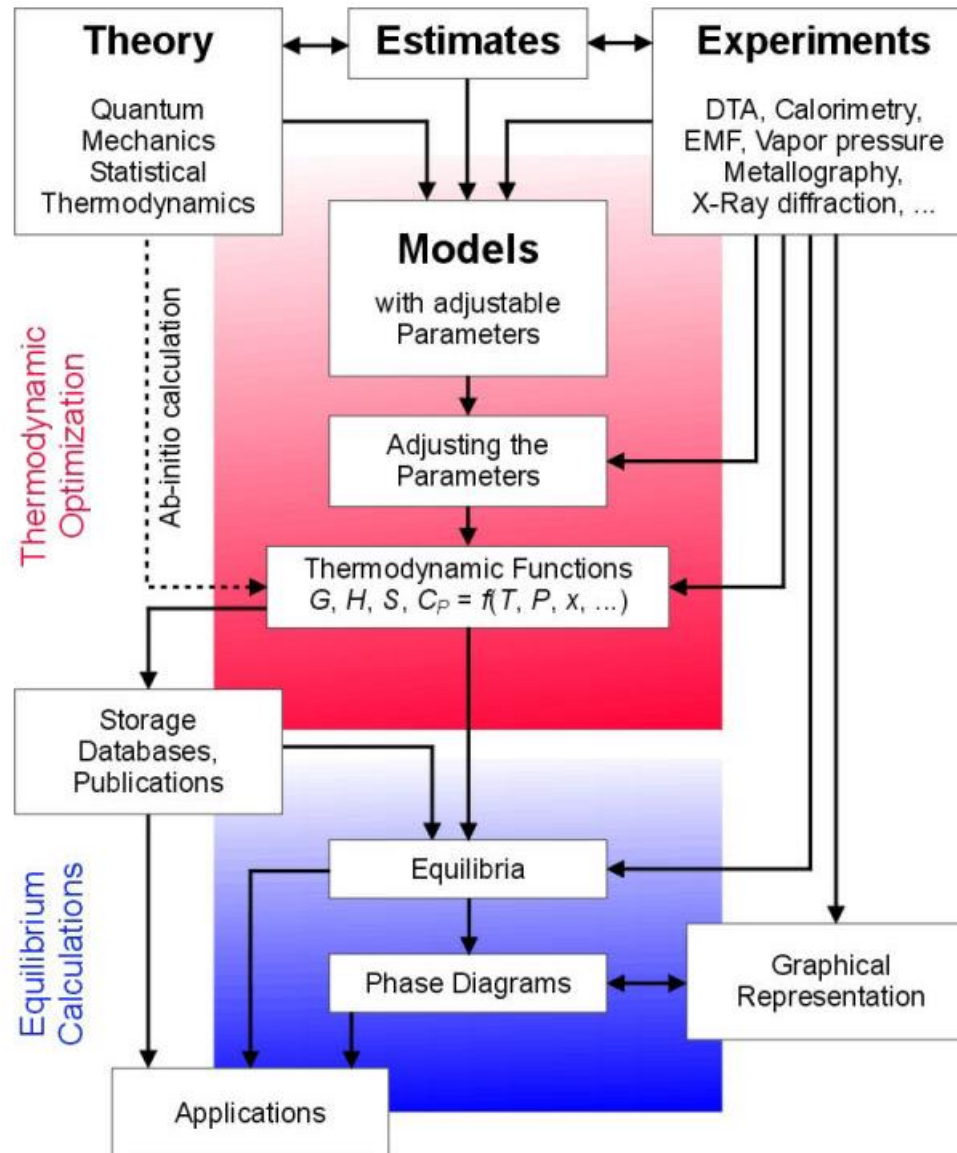


- Databases are produced by critical assessment of experimental data and optimization of model parameters (the CALPHAD method).
- PARROT in Thermo-Calc Classic can be used as a tool in this process.

Description of the Gibbs energy for each phase  
 $G_{\phi} = G_{\phi}(x, T, P)$  is stored in the database

- 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).

# The CALPHAD method.



## Thermochemical data

- Calorimetric data – Enthalpy of formation, Enthalpy of mixing, Enthalpy of transformation
- EMF, Knudsen cell data – Chemical potentials, Activities
- Partial pressure – Activities
- DSC – Heat content, Heat capacity, Enthalpy of transformation



## Phase diagram data

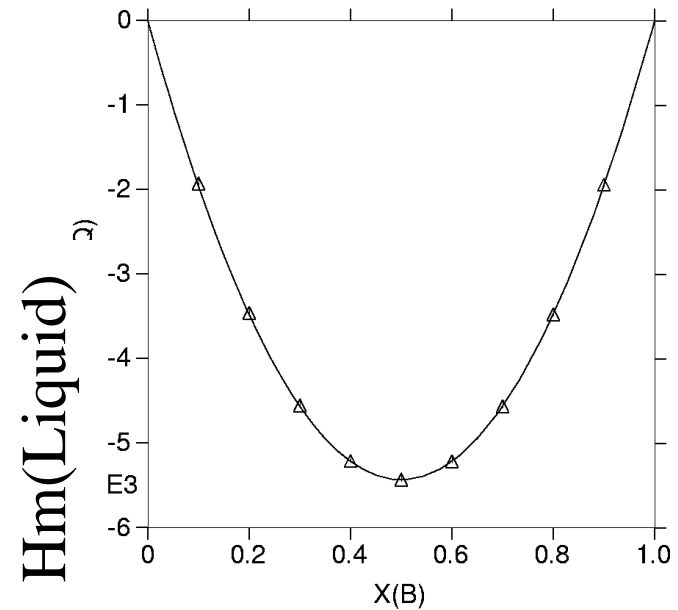
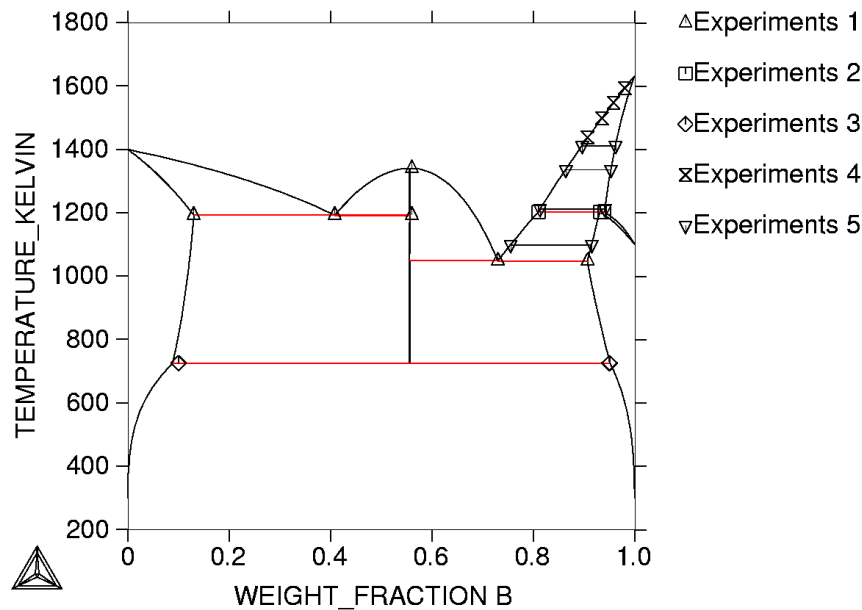
- Thermal analysis – Start and end temperatures of transformation
- Microscope – Identification of phases, amount of phases
- X-ray – Phase identification, lattice parameters
- Microprobe – Phase identification, composition of phases
- X-ray and neutron diffraction – site occupancy

## Two types of data

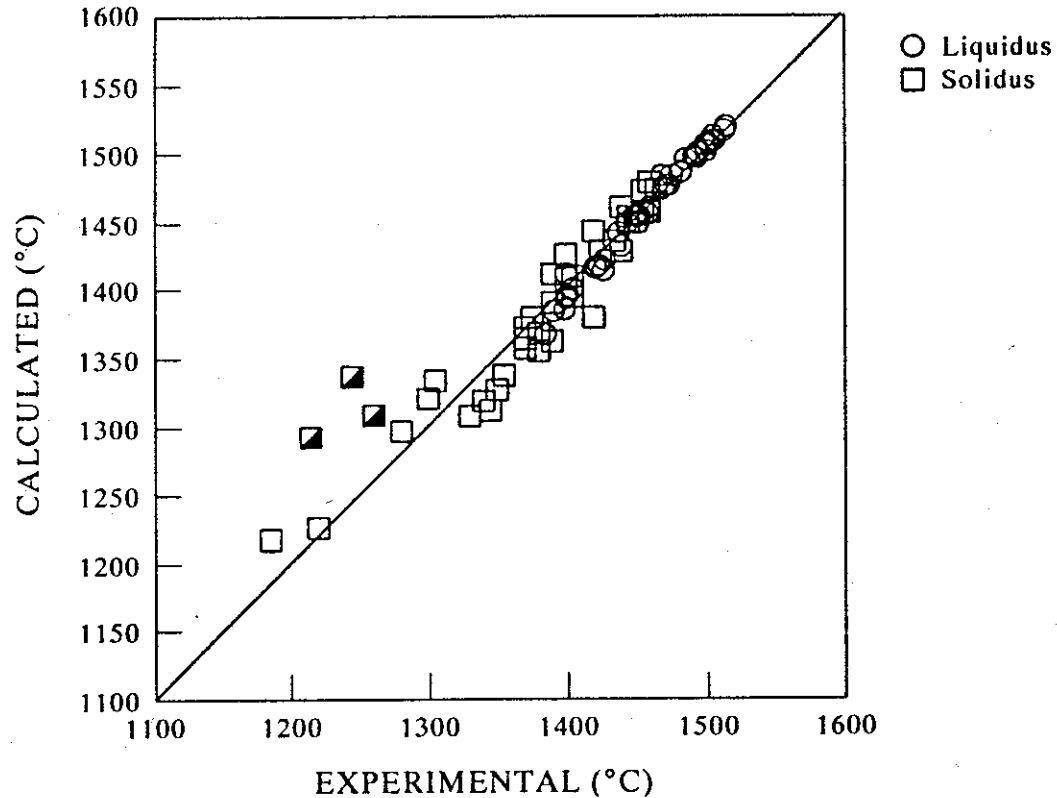
- Basic thermodynamic and phase equilibrium data – the building blocks of thermodynamic databases
  - Experimental
    - Phase equilibrium (phase diagrams) for binary and ternary system (liquidus/solidus/phase boundary)
    - Thermodynamic data for compounds/stoichiometric phases
    - Activity measurements etc
  - Theoretical
    - Estimation and Ab initio calculations
  
- Higher order (multi-component data) – validation for alloys etc
  - Experimental
    - Cp, liquidus/solidus/phase boundary data etc for “real” alloys
    - Volume fraction of carbides etc

# Binary and ternary systems

- Normally collected from the literature
- Reliable data is selected and critically assessed
- Both phase diagram data or thermodynamic data ( $\Delta H, C_p \dots$ ) can be used



# Higher order systems: Real alloys for validation



**Figure 10.37** Comparison between calculated and experimental (Jernkonteret 1977) solidus and liquidus values of a range of steels.

From: Saunders & Miedownik: "Calphad -a comprehensive review"

# Utilizing first principles approaches

High-throughput ab-initio capacity and infrastructure for piping data into CALPHAD database development:



# MedeA



# Molar Volume of Liquid $\text{Al}_{1-x}\text{Cu}_x$

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

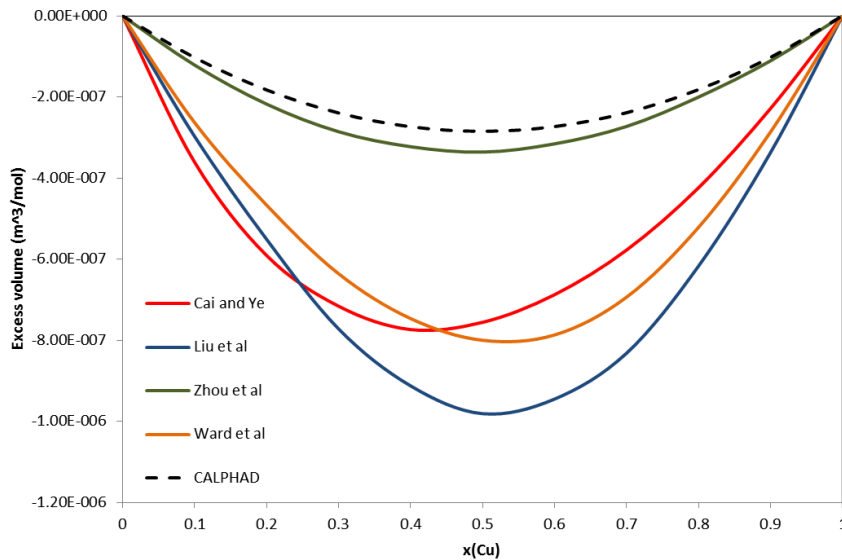
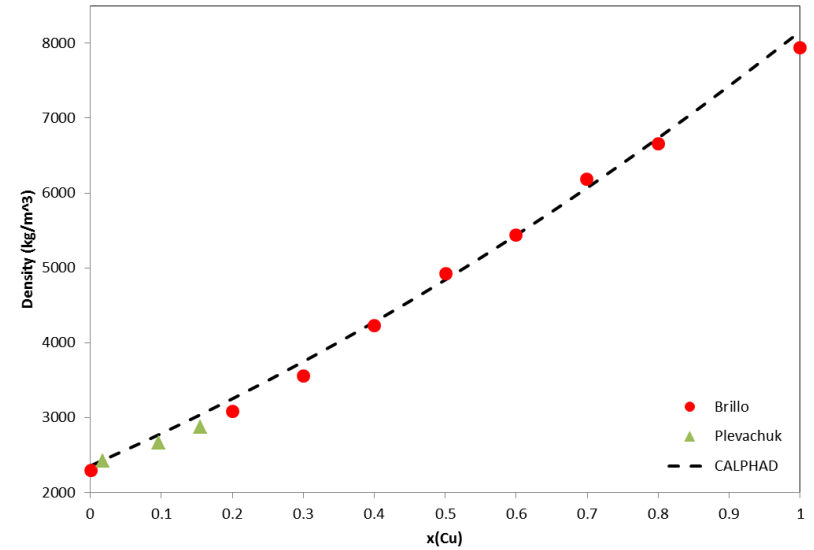
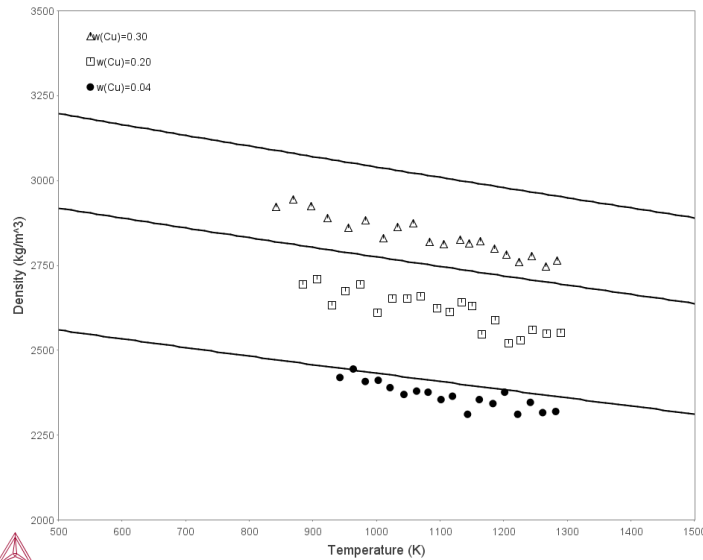
Fitting to the data by Brillo et al gives a negative excess volume

It is impossible to simultaneously fit both sets of data

Question: Which set of experimental data should we trust?

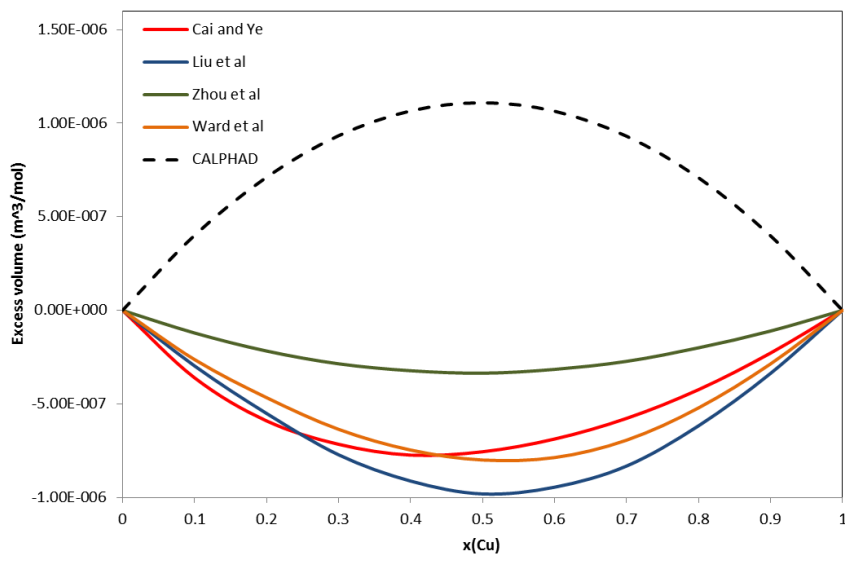
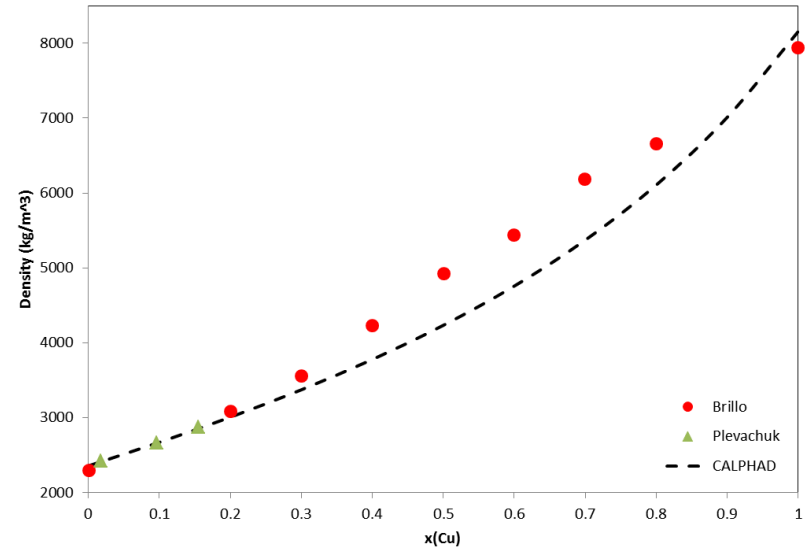
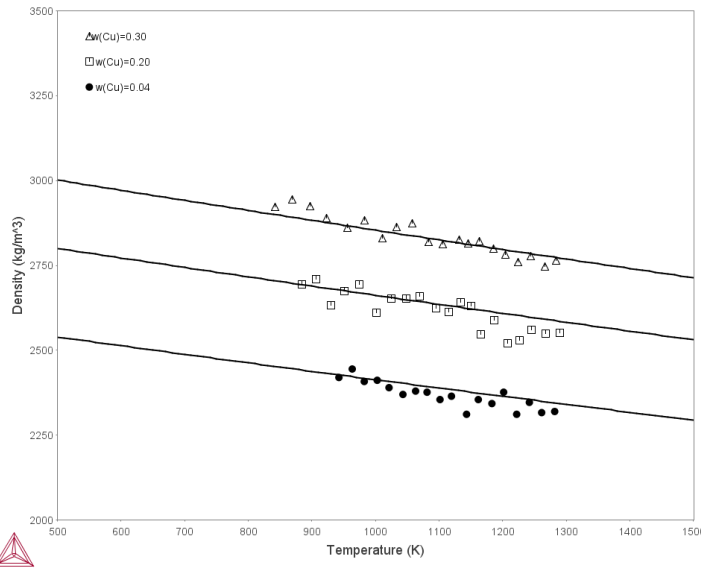


# Case I



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

# Case II

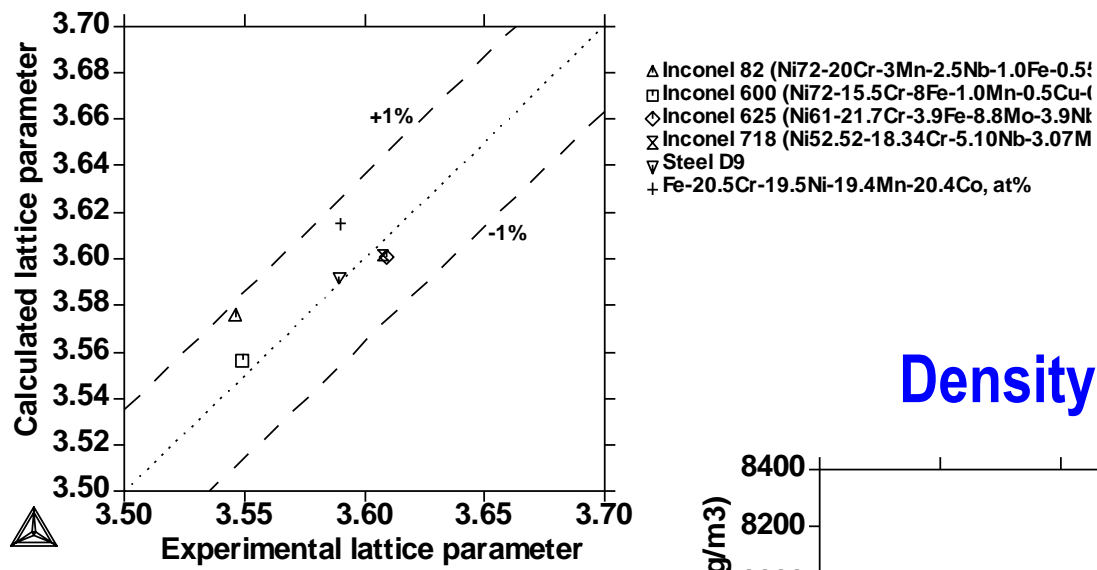


Fitting to the data by Plevachuk et al gives a positive excess volume, which contradicts MD results for the liquid Al-Cu alloy. Therefore, it is suggested that the experimental data from Brillo et al. be used for CALPHAD assessment.

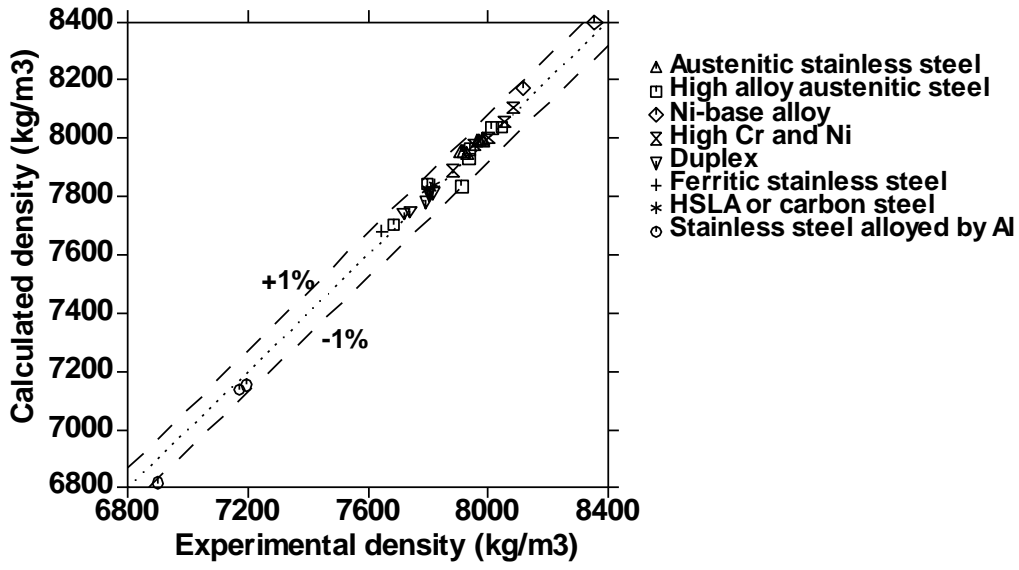


# Density and Lattice parameter

## Lattice parameter of Ni-base alloy

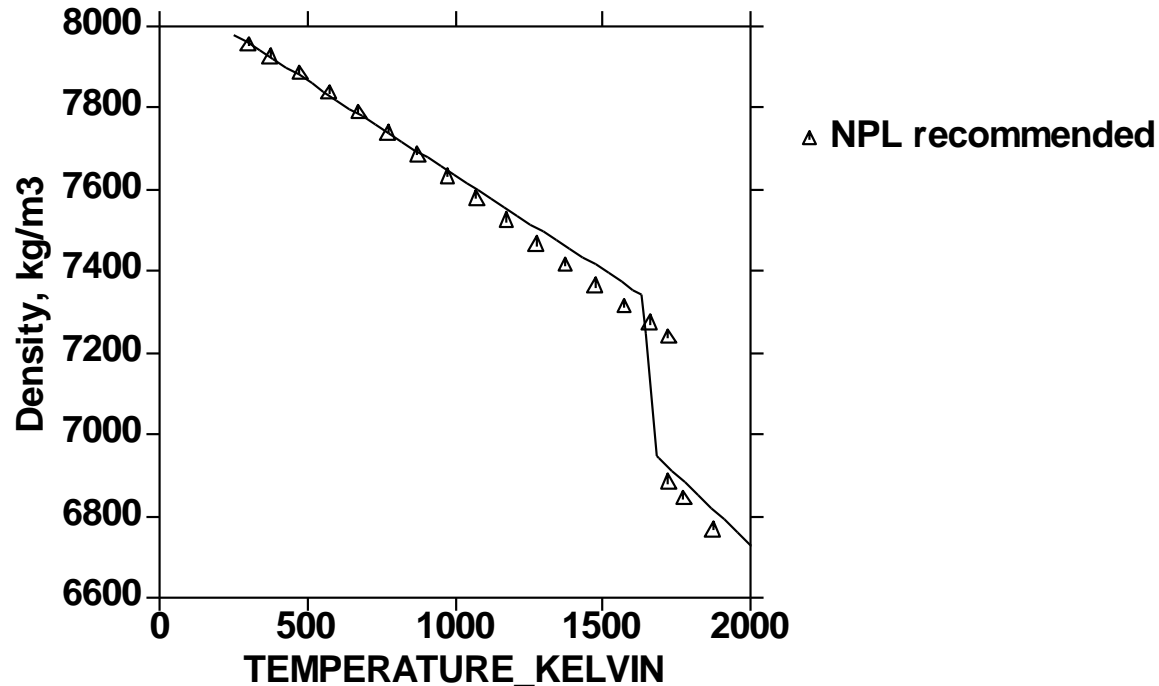


## Density of steels



# Density of Stainless steel

Steel 316: Fe-12Ni-17Cr-1.0Si-2.0Mn-2.5Mo-0.3Cu-0.08C (wt%)



Combining with Scheil or DICTRA simulation, density variation during solidification can be calculated more properly.

# Selecting the right database(s) (1)

Three most common types of databases:

**Substance database** (e.g. SSUB5, 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. TCFE9, TCNI8, SSOL6, TCOX7, 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

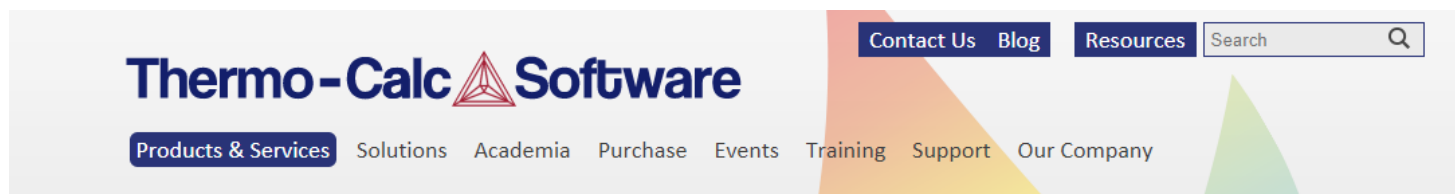
**Aqueous databases** (e.g. TCAQ3, AQS2):

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

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

# Selecting the right database(s) (2)

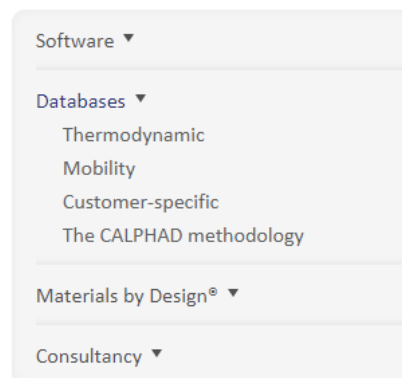
For a list of available thermodynamic and mobility databases refer to the database overview or [www.thermocalc.com](http://www.thermocalc.com)



## Databases

*The quality of the predictions is strongly dependent on the quality of the database. This means that the database is as important, if not even more important, than the software using it.*

Thermo-Calc Software has long experience in the field of CALPHAD and database generation, and possesses a highly qualified team of people working on database development. With our databases, you can rest assured that you are working with the most advanced databases available.



### Thermodynamic Databases

There is a vast selection of thermodynamic databases for different types of materials. Find out which ones suit your needs »



### Mobility Databases

Mobility databases are used when performing kinetic simulations with DICTRA or TC-PRISMA, but can also be used together with our SDKs. [Learn more »](#)



### Customer-specific Databases

If you can't find a database that suits your needs »

[Database Overview »](#)

# Selecting the right database(s) (3)

Most of the solution databases have extended information

## Nickel-based Alloys

### TCNi8.1:

TCS Ni-based Superalloys Database, v8.1



[Extended Information](#)

## Aluminium-based Alloys

### TCAL4:

TCS Aluminium-based Alloys Database v.4



[Extended Information](#)

## Magnesium-based Alloys

### TCMG4:

TCS Magnesium-based Alloys Database, v4



[Extended Information](#)

## Copper-based Alloys

### TCCU2:

TCS Cu-based Alloys Database v2



[Extended Information](#)

## High Entropy Alloys

### TCHEA2:

TCS High Entropy Alloys Database v2



[Extended Information](#)

# Selecting the right database(s) (4)

These contain a list of binary and ternary systems evaluated

Assessed Binary Systems in Full Range of Composition and Temperature

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

# Selecting the right database(s) (5)

And validation

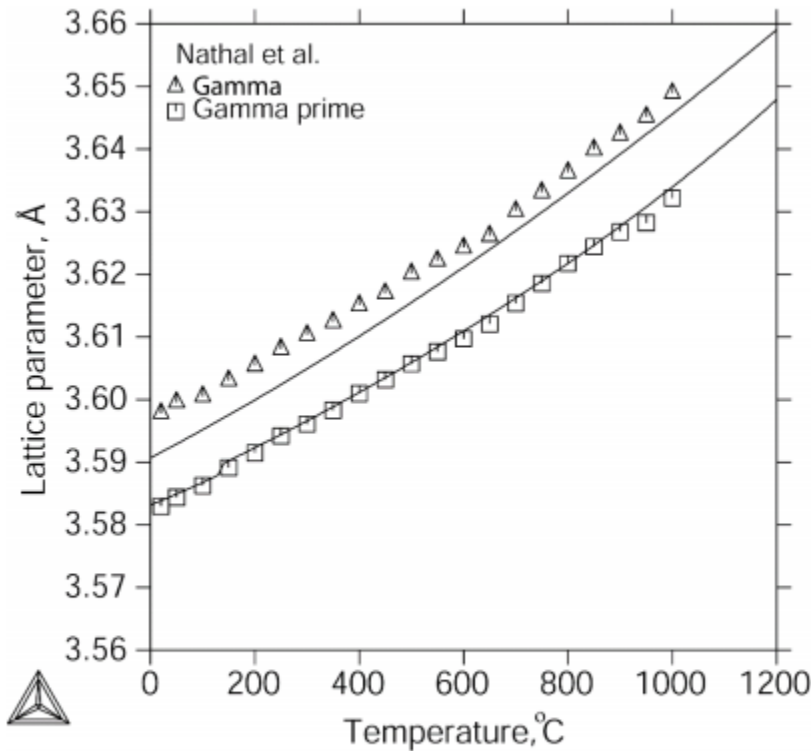


Figure 10. Predicted  $\gamma/\gamma'$  lattice mismatch of a Ni-0.6Mo-0.92Ta-12.5Al-1.83Ti-10.5Cr-3.3W (at. %) compared to an experimental determination by Nathal et al. [19].

# Selecting the right database(s) (6)

To choose the correct database:

1. What kind of material are you working with? Is it an alloy (e.g. a steel, a Ni alloy, Al alloy, etc) or is it a refractory oxide system, a slag, an aqueous system? Often the most common materials have a specific database available.
2. How well is your system described. Create a matrix of elements like on slide 90 and check off how many binary (and ternary) systems are described for your material. The more, the better.
3. For systems not covered can you append any data from another database?



# Appending database(s) (1)

You may need to append databases for the following situations:

1. You want to make a kinetic calculation using DICTRA or TC-PRISMA and you need to append the mobility data to the thermodynamic data.
2. You want to make a calculation for a system that is more complex than say for just a regular alloy. For example appending data from a substance database to simulate oxidation in a multicomponent alloy where you would append the gas and oxide data from the substance database with the alloy data from the alloy database. Or you want to make an aqueous corrosion calculation where you would append data from the aqueous database with data from the alloy (and possibly substance databases).

## Appending database(s) (2)

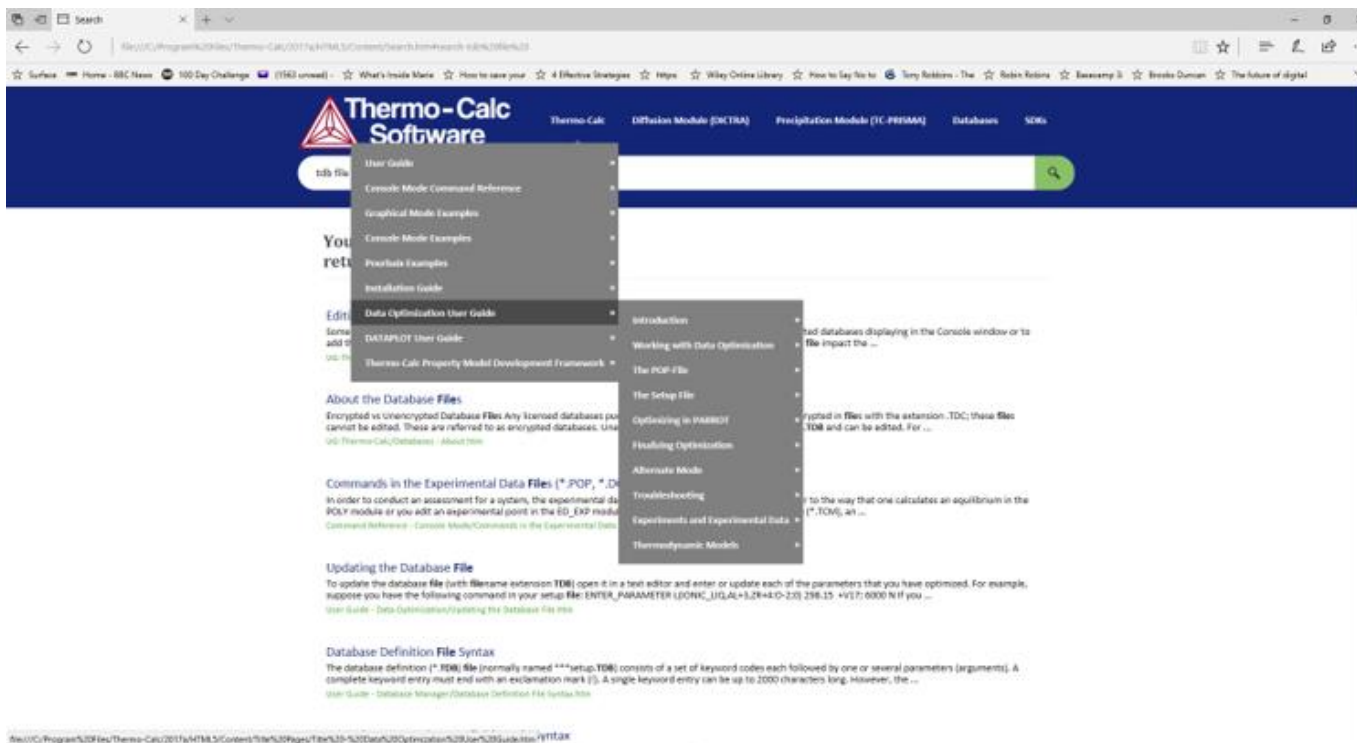
Be careful when appending databases:

1. You cannot easily combine data from one solution database to another solution database for the same phase, e.g. adding a binary description from SSOL for FCC to TCFE. You will simply overwrite the phase description from TCFE. You need to append data with a unique phase name.
2. When appending data from e.g. SSUB to a solution database you will want to unselect or reject the condensed phase data that is better described in the solution database (e.g. the data for the elements for example or intermetallic compounds, such as carbides, that are included in the solution database).
3. The order in which you append matters. You are adding (or overwriting data) to the database to which you are appending. If you append TCFE with TCOX add TCFE second because you want the solution phase for the alloy to be correct.

# Creating your own database(s) (1)

Thermo-Calc does allow the reading in of user's own databases which can be created in an ASCII text file format. These need to be created using the CALPHAD approach which is beyond the scope of this introductory training course.

The format of the user's own database is described in the data optimization and user guide



The screenshot shows the Thermo-Calc Software website. The navigation menu includes: Thermo-Calc, Diffusion Module (DICTRA), Precipitation Module (TC-PRISMA), Databases, and SOLID. A search bar is located in the top right. The main content area is partially obscured by a dark overlay containing a list of links: User Guide, Console Mode Command Reference, Graphical Mode Examples, Console Mode Examples, Precalcs Examples, Installation Guide, Data Optimization User Guide, DATAPLOT User Guide, Thermo-Calc Property Model Development Framework, Introduction, Working with Data Optimization, The PCP File, The Setup File, Optimizing in PHAROT, Heatmap Optimization, Aberrate Mode, Troubleshooting, Experiments and Experimental Data, and Thermodynamic Models. Below the overlay, the page content includes sections for 'About the Database Files', 'Commands in the Experimental Data Files (\*\_POP, \*\_D)', 'Updating the Database File', and 'Database Definition File Syntax'.

# Challenge 1: Completeness of data

- ❑ Many systems have yet to be critically assessed in terms of a CALPHAD assessment to determine the underlying thermodynamics for binary systems, let alone ternaries.
- ❑ The **ASM Alloy Phase Diagrams Center** allows subscribers to *explore, search and view* more than 34,000 binary and ternary phase diagrams and associated phase data for more than 6200 systems from their Web browsers.
  - But you cannot make calculations or extrapolate to alloys
- ❑ In contrast the SSOL5, the latest version of the **SGTE Solution database** has assessments for 414 binary systems and 127 ternary systems.
- ❑ Ternary compounds cannot exist in a binary system, so ideally the ternaries should also be assessed.

# Challenge 2: Basic composition and temperature dependent data

❑ Extending CALPHAD requires good quality, basic composition and temperature dependent data for i) binary and ii) key ternary systems, for:

- Diffusion data to determine atomic mobilities
- Volume data
- Interfacial energies (coarsening experiments)
- Other properties ?

❑ While industry collected data (for multicomponent alloys) is useful and critical for validation and identifying problems with databases, it is less useful for database development since this requires data for very basic systems which are of less industrial importance and more basic research. Identifying better ways of using industry collected data should be explored though.

## Challenge 3: Low and high temperature data

- ❑ Historically CALPHAD thermodynamic data was based on assessing experimental data that was believed to have reached equilibrium (most typically at high temperature, or fast diffusing systems).
- ❑ Low temperature data (important for precipitation kinetics) are mostly based on extrapolation from high temperature to low temperature (although being supplemented more by ab initio data now).
- ❑ Very high temp data can also be a challenge though – high melting systems are difficult to measure experimentally, and not much is known about e.g. volumes or diffusion in liquids for example – mostly estimated data.

# Challenge 4: Maintaining and updating databases

- It is difficult and time consuming to change unary (data for elements or end members) and even some key binary systems because of the impact that this has on the higher order systems.

# Challenge 5: You don't know what you don't know

- ❑ G phase, Z phase have recently been added to some thermodynamic databases, but these slow precipitating phases were not included in the databases previously because no one had observed them – no one does experimental heats for 20-30 years!
- ❑ CALPHAD can only predict the formation of what is included in the databases. Ab initio can help supplement this, but...
- ❑ Catch 22 – even if CALPHAD had included these in the databases and the phases had been predicted a lot of people would not have believed they would form, without experimental evidence.



## Challenge 6: Data for metastable phases

□ Metastable phase data is non-equilibrium and tends to be obtained by inference – cannot measure directly which presents challenges. But is important for processing type simulations.

# Challenge 7: Quantifying uncertainties

- ❑ One of the strengths of CALPHAD is that it is a self consistent framework that takes many different kinds of experimental (and ab initio) data. So outliers tend to stand out in the data sets and can be investigated more closely and in some cases rejected. So there is a self validation going on here.
- ❑ CALPHAD captures the uncertainty in the experimental database on which an assessment is built.
- ❑ But it does not quantify that uncertainty. Nor is it able to extend this uncertainty to a prediction for the multicomponent system.
- ❑ CALPHAD also does not really know if it is in assessed space or not. Is a calculation based on binary systems alone good enough? It might be if there are no ternary compounds, but we don't know that.

## Challenge 8: Good quality consensus data for multicomponent alloys - validation

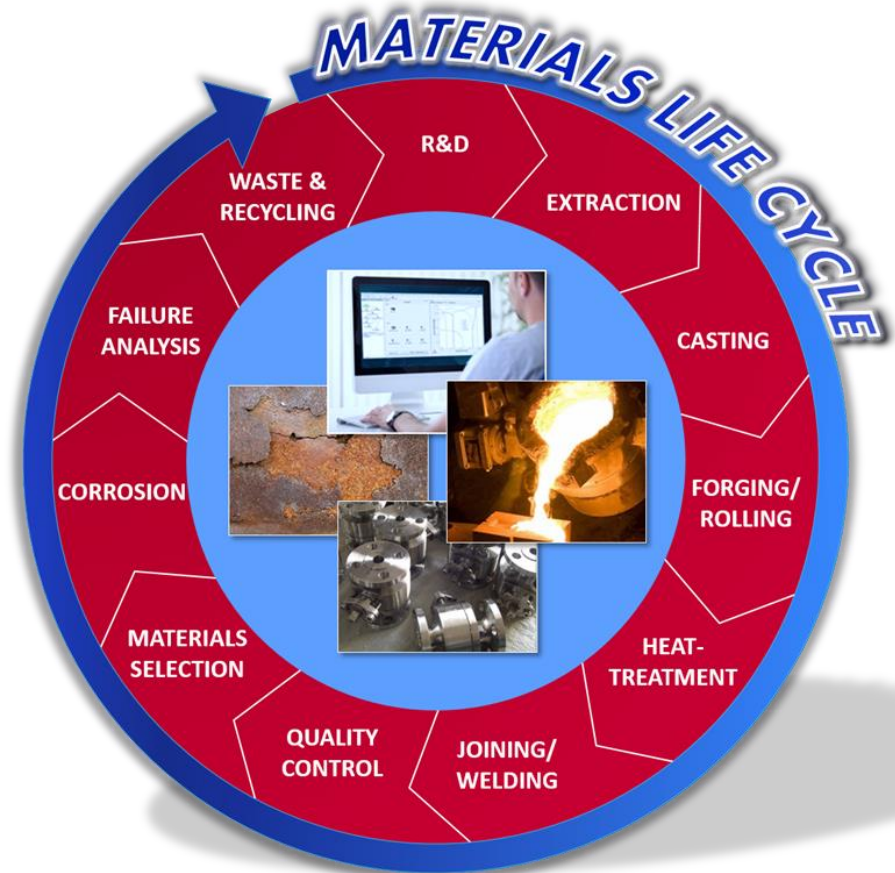
- ❑ CALPHAD uses multicomponent (alloy) data to validate the databases, not fit them! But finding good quality data, where consensus has been reached on what is a good validation set would be useful (like a standard or an agreed benchmark) for a range of different alloys within a given alloy type (e.g. steels, Ni-superalloys, Al alloys, etc).
- ❑ Not so much data like this is published, but industry probably has a lot of data, even for non-proprietary alloys, or alloys they are willing to share, that show the scatter in the experimental data. It would be very beneficial to have a public database like this with meta data (actual compositions as opposed to nominal for example).

# Challenge 9: What makes good experimental data

- For thermodynamic / phase equilibria assessments, experiments need to reach equilibrium otherwise you can get incorrect volume fractions, metastable phases present etc. At lower temps, kinetics can be very slow.
- Reproducibility. Few experiments are repeated sufficiently to assess the reproducibility.
- Accuracy: Liquidus as an example is defined as the formation of the first solid. But what if the first solid is a very small fraction (e.g. a metal boride of  $1\text{E}-05$  moles in a liquid Ni superalloy)?
- For multicomponent validation (in particular) knowing the specimen composition accurately (not enough to say it's an alloy of a certain grade with a nominal composition).
- Contamination: Interactions between samples and the containment/crucible materials
- Open vs closed systems – particularly important for volatile systems and incongruent vaporization.

# Examples with application to the materials life cycle

*To provide computational tools in the field of materials engineering that allow for faster, cheaper and more sustainable innovation, development and production of both materials and components.*

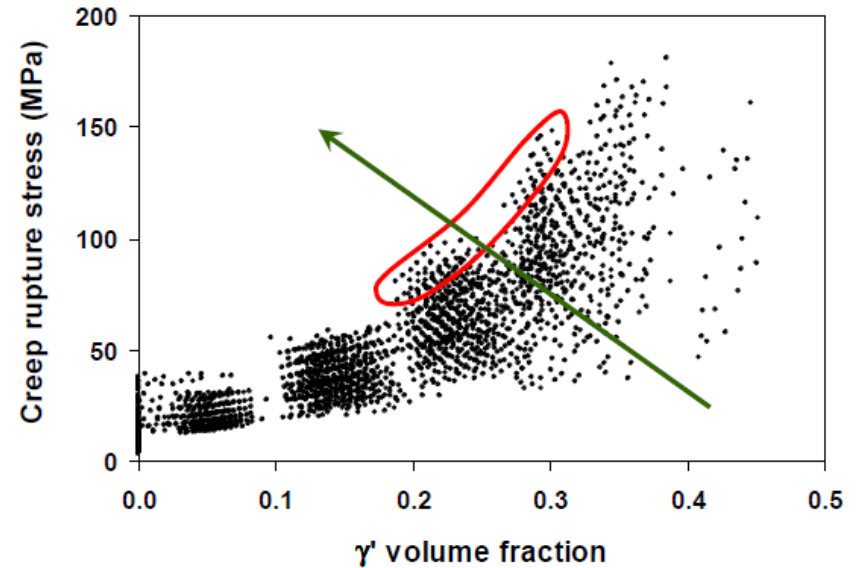


For more examples, we encourage you to do an application specific literature search

# Applications to R&D

Examples include:

- Considering the chemical variation of the alloy on the phases that form, the amounts and compositions of those phases and the phase transformation temperatures.
- Pre-screening large numbers of potential candidate compositions to guide experiments.
- For cast materials, predicting how likely the material is to segregate and how long homogenization treatments could take.
- Optimizing heat treat schedules for the alloy to balance properties, such as the formation of strengthening precipitates versus corrosion resistance, as one example.



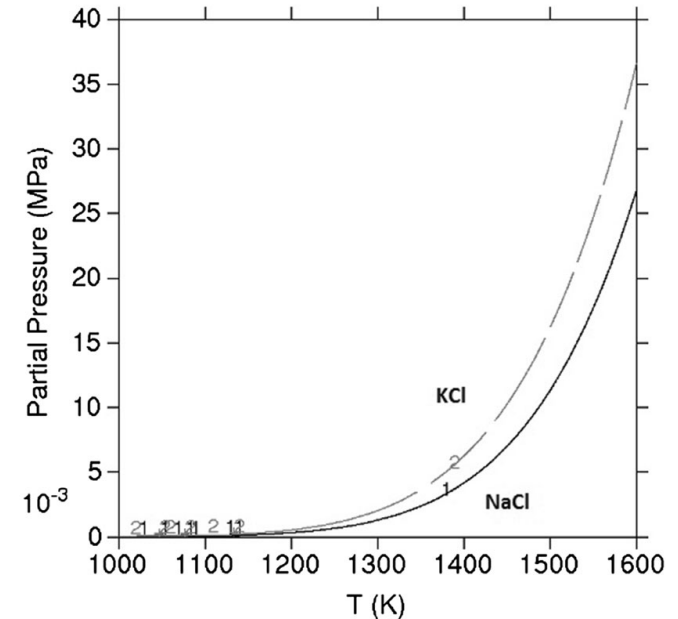
Optimization of an alloy composition for the design of weldable and creep resistant superalloys using Matlab, TC-Matlab toolbox and neural net models. Over 16,000 compositions assessed. (Tancret, 2009)

# Applications for Extraction

Examples include:

- Developing and optimizing slag systems for both ferrous and non-ferrous applications
- Modelling interaction between slag and liquid metal and prediction of inclusion formation, partition coefficients, solidus and liquidus temperatures, etc.
- Simulating dephosphorization and desulfurization
- Performing relevant heat, mass and thermodynamic calculations for the extraction of base metals
- Calculation of predominance area diagrams (for example, Fe-H<sub>2</sub>O system)

THERMO-CALC  
DATABASE:SSUB3  
P=1E5, N(CL)=2, N(K)=1, N(NA)=1;



Partial pressure of NaCl and KCl versus temperature ( $P_{\text{total}} = 10^5$  Pa; equimolar mixture of NaCl-KCl)

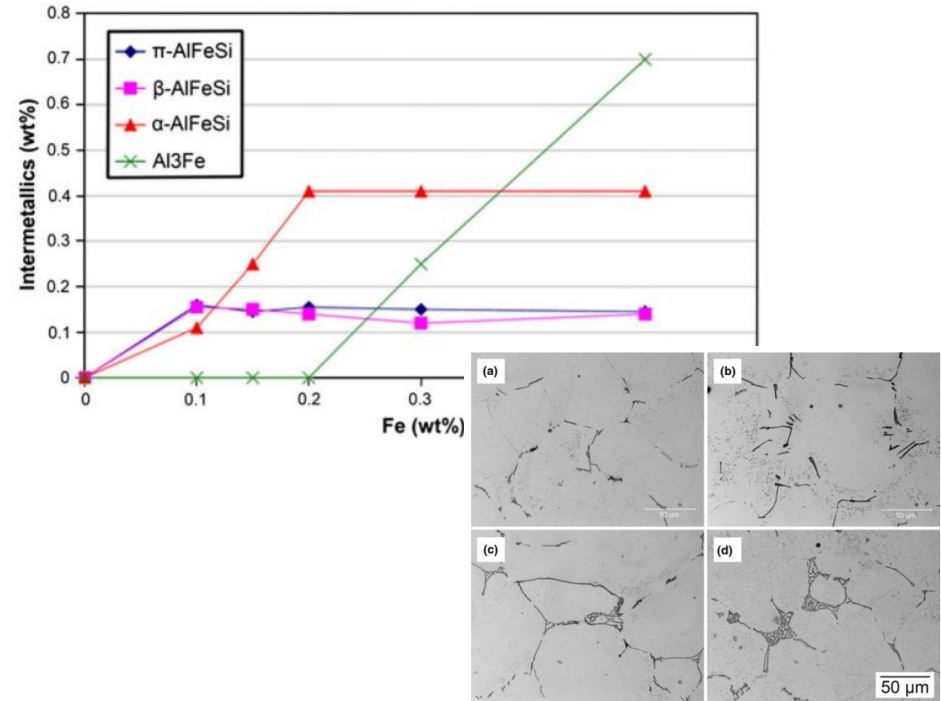
This type of information is useful in optimizing removal of salts from white/black dross during aluminum production

Beheshti, Reza, et al. *JOM* 66.11 (2014)

## Applications to Casting

Examples include:

- Calculation of equilibrium and non-equilibrium solidus/liquidus temperatures
- Incipient Melt temperatures
- Fraction solid curves (under equilibrium and non-equilibrium conditions)
- Micro-segregation predicted by Scheil solidification simulations, including partial equilibrium in the liquid and solid for elements identified by the user as fast-diffusers
- Calculate latent and specific heat
- Prediction of shrinkage during solidification/cooling



Top: The amount of the Fe-containing intermetallic phases at the end of solidification as a function of alloy Fe content, as predicted by Thermo-Calc

Bottom: Optical micrographs showing the typical morphology of intermetallic particles in the 6060 alloys containing (a) 0.1, (b) 0.2, (c) 0.3, and (d) 0.5 wt pct Fe.

Authors used TEM to identify phases, and found broad agreement with Thermo-Calc predictions.

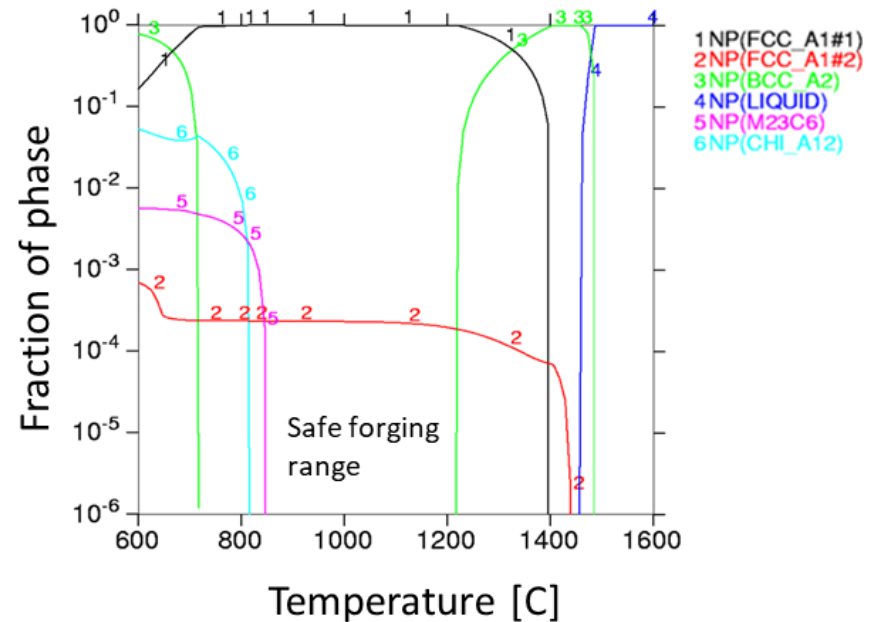
Sweet, L., et al. Met Trans A. (2011).



# Applications to Forging/Rolling

Examples include:

- Establish composition ranges which give the widest precipitate free region over the widest range of temperatures possible
- Predict formation of precipitate phases within an alloy as a function of composition and temperature, along with the amounts of those phases and their compositions.
- Simulate the solutionizing kinetics; the time required to dissolve precipitates into the solution phase.
- Simulate the changes in size distribution as a function of chemistry, temperature and time to establish the sensitivity of the precipitate size distribution to these parameters.



Phases vs Temperature for a Supermartensitic stainless steel, used to determine precipitate free region for optimal forging.

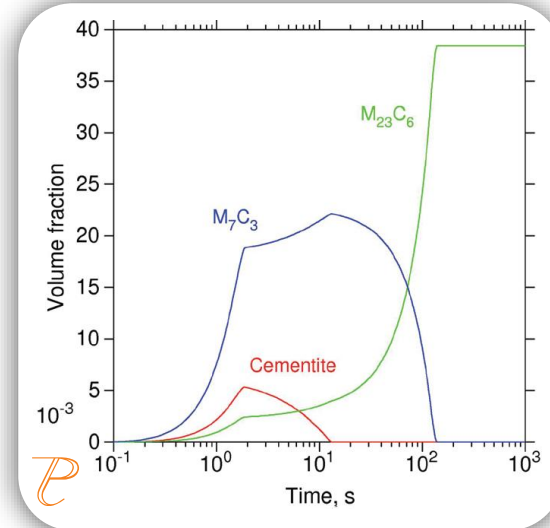
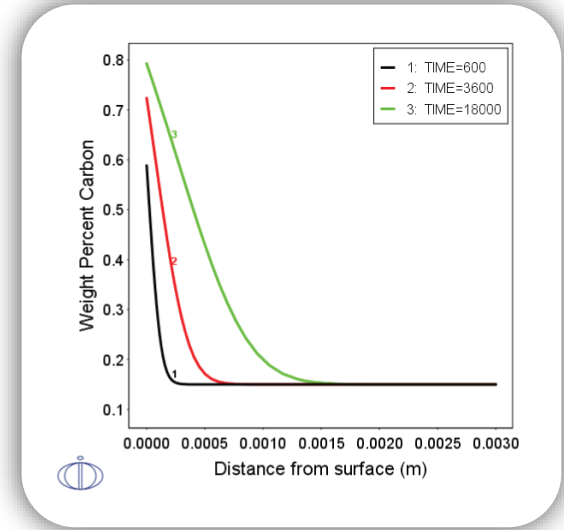
Courtesy André Costa e Silva

# Applications to Heat Treatment

Examples include:

- Calculate furnace activities based on gas composition, temperature and pressure
- Predict the amount and composition of precipitate phases as a function of alloy chemistry and process temperature
- Plot multicomponent phase diagrams, including Lehrer diagrams, for alloys that allow a quick overview of optimal processing conditions
- Simulate the diffusion of elements in multicomponent alloys as a function of chemistry and temperature
- Simulate concurrent nucleation, growth, dissolution and coarsening of precipitates as a function of alloy chemistry, temperature and time

Carbon Depth profiles at different times during carburization of a low alloy steel – Simulated w/ DICTRA



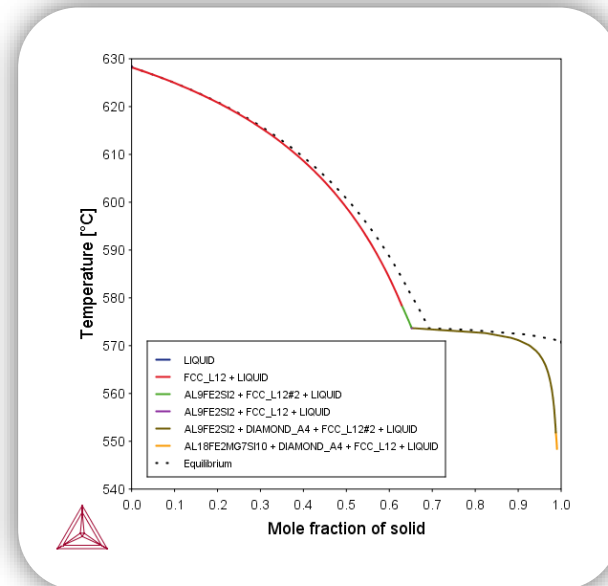
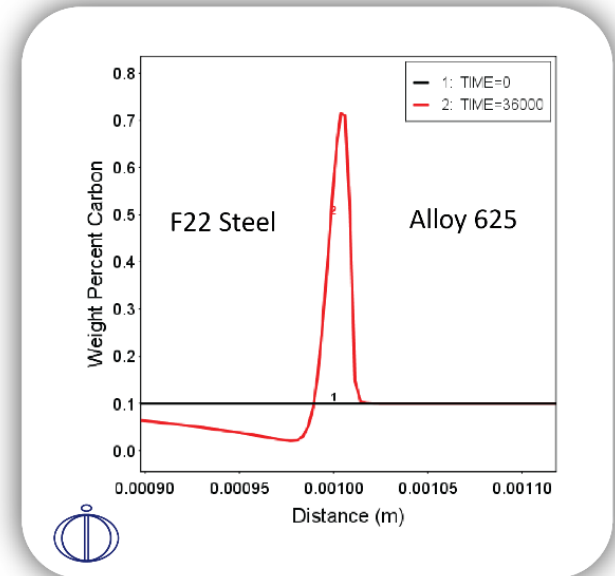
TC-PRISMA simulation of the stable/metastable carbide precipitation sequence in 12Cr martensitic stainless steels

# Applications to Welding + Additive

Examples include:

- Prediction of microsegregation during solidification using Scheil calculations
- Prediction of heat affected zone grain boundary liquation
- Understanding phase stability in the heat affected zone for dissimilar materials and dilution effects
- Identifying potential filler wire or powders, and dilution effects with the base metal
- Predicting thermodynamic properties such as heat evolved, specific heat latent heat during solidification that can be used as input parameters to welding simulation models

DICTRA prediction of carbon accumulation at the fusion boundary of a dissimilar metal weld during PWHT



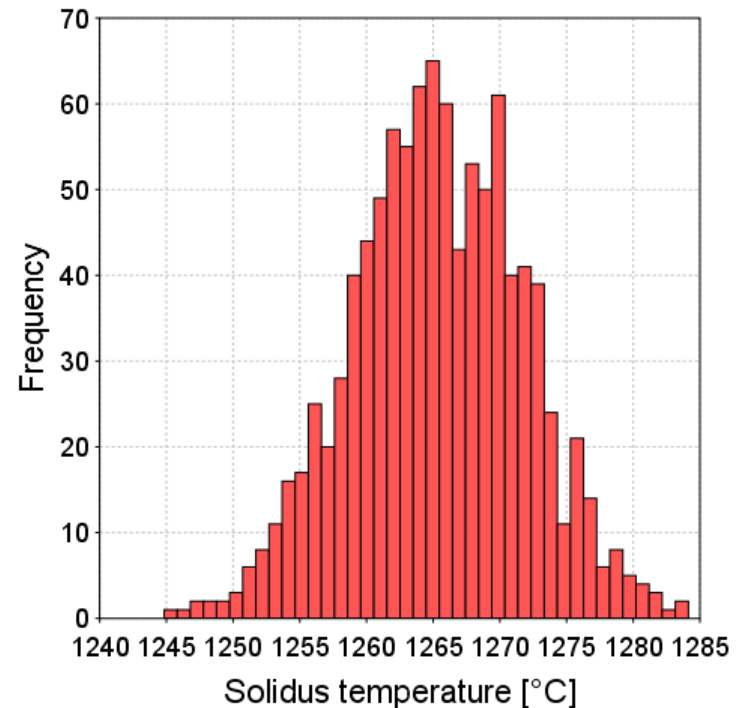
Scheil  
solidification  
simulation of  
aluminum 4340

## Applications to Quality Control

Alloys typically have a nominal or target chemistry and an allowable tolerance range for each element.

Determining the sensitivity of a particular property, such as the solvus temperature of a given phase, for example, can be done for all combinations of chemistry within the allowed range, thus establishing a range for that given property rather than a single value based on nominal chemistry.

Determining tail effects due to variation within chemistry can require many hundreds of experiments, but a computational approach can provide insight into these ranges in an efficient manner and allow customers to establish operational windows, both in terms of allowable chemistries and temperatures, during various stages of a process.

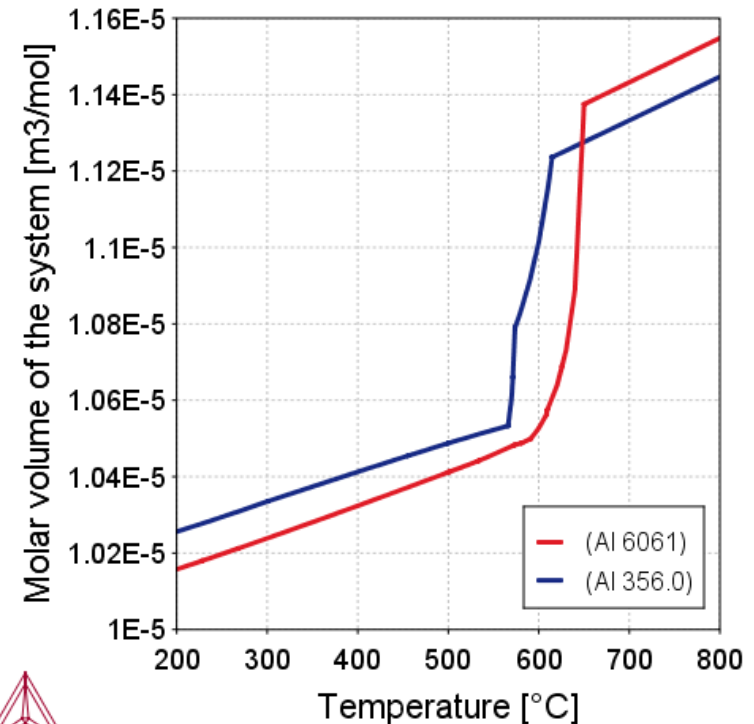


Variation in solidus temperature over the normal composition range for Alloy 718 – 1000 compositions normally distributed across the allowed min/max

## Applications to Materials Selection

Examples include:

- Optimizing the composition of a material to give the required microstructure in terms of amounts of phases formed, e.g. precipitation hardening phases, while balancing this against other property requirements.
- Predicting the phases that could form at the interface in dissimilar material welds
- Predicting the long term stability of a material, the formation of life limiting phases and corrosion products under operational conditions.
- Considering reactions between a material and its containment, e.g. liquid – crucible reactions in a ladle.

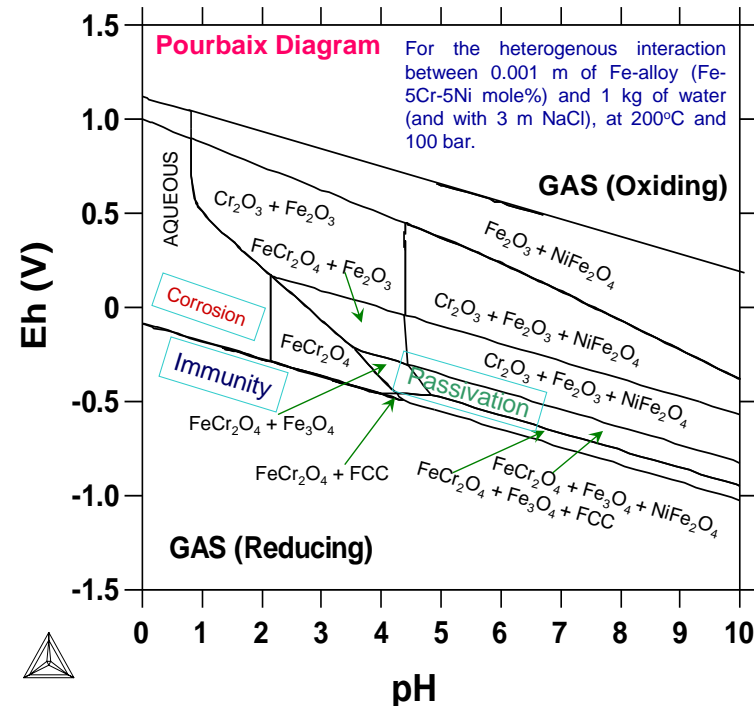


Comparison of molar volume in two Aluminum alloys – used to compare shrinkage during solidification/cooling

# Applications to Corrosion

Examples include:

- Calculation of Pourbaix diagrams for multicomponent alloys systems in aqueous environments
- Predict the amounts and compositions of phases for metal-aqueous, metal-gas and metal-molten salt systems.
- Simulate degradation of protective NiAl coatings for Ni-based superalloys
- Predicting oxide growth on metal surfaces where diffusion through the metal is the rate limiting step
- Calculate stable oxide phases as a function of oxygen partial pressure

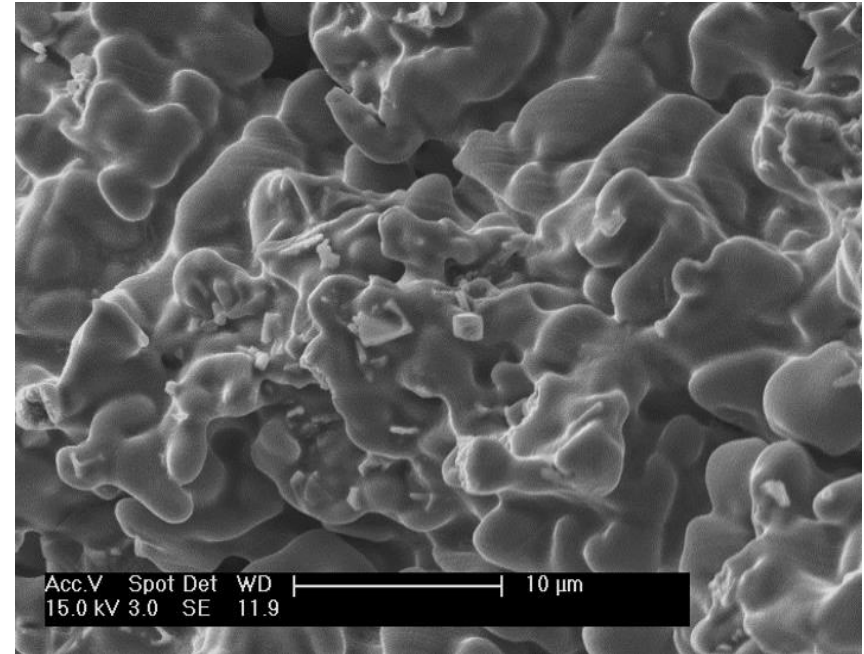


Calculated Pourbaix diagram of a 5Cr 5Ni steel in a 3M NaCl solution at 200°C and 100bar.

## Applications for Failure Analysis

Materials can fail for a number of different reasons and sometimes the reason for those failures can be attributed to an underlying aspect of the chemistry of the material, for example the formation of a deleterious phase, a life limiting phase, a lower than expected phase transformation temperature and so forth.

Thermo-Calc can complement post-failure testing, microstructural analysis, etc., in order to give better insight into the potential influence of chemical changes on the failure and insight into how chemical changes to the composition or processing conditions can be made to avoid such failures in the future.



Fracture surface of a solidification crack in a Ni alloy. Thermo-Calc predicts Ti(C,N) at end of solidification. Particles on fracture surface likely Ti(C,N) based on EDS results and prediction

Courtesy Dr. Carolin Fink and Micheal Orr – Ohio State University

# 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.

For more than 20 years CALPHAD based tools have been used to accelerate alloy design and improve processes with applications throughout the materials life cycle.



# Questions?