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

Paul Mason

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

Goals of this webinar

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.

During this webinar, 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 including steels and Ni-base superalloys.

Outline

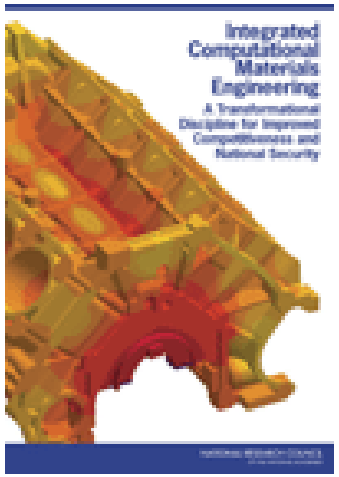
There are three main sections to this webinar:

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?



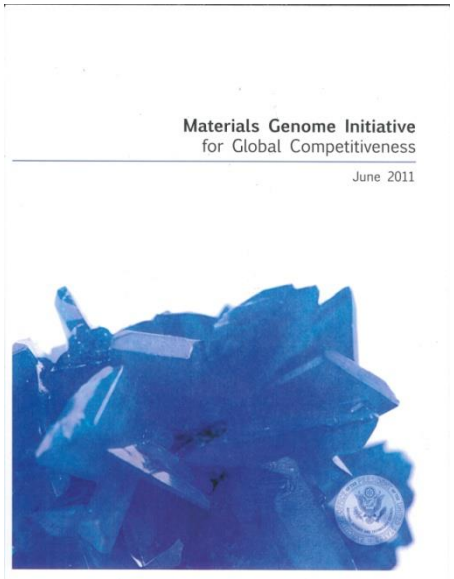
The National Academies Press, 2008

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.

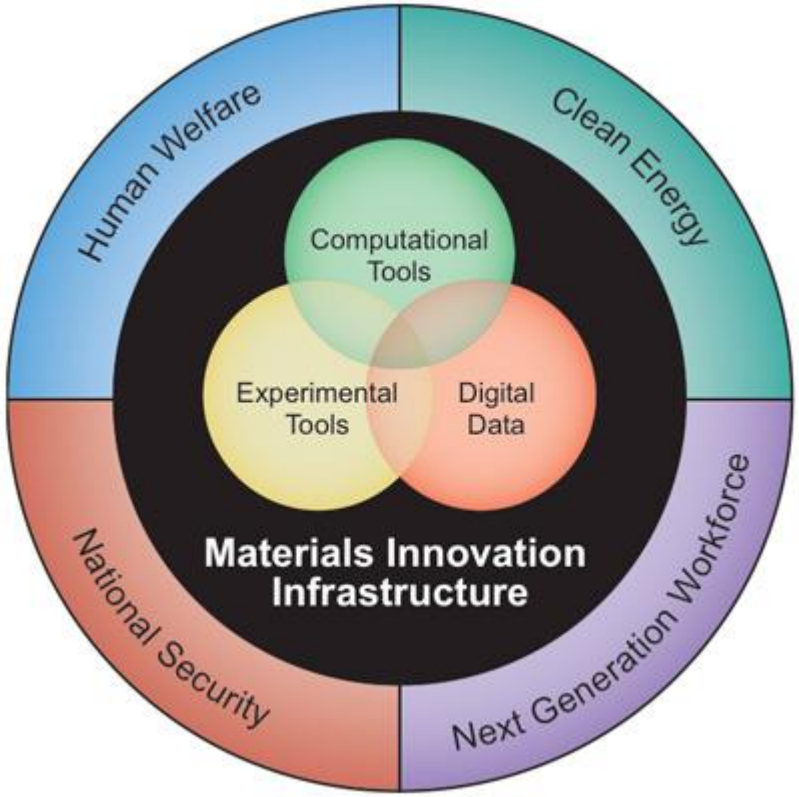
Focus is on the materials, i.e. understanding how processes produce material structures, how those structures give rise to material properties, and how to select materials for a given application. This report describes the need for using multiscale materials modeling to capture the process-structures-properties-performance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

What is MGI?



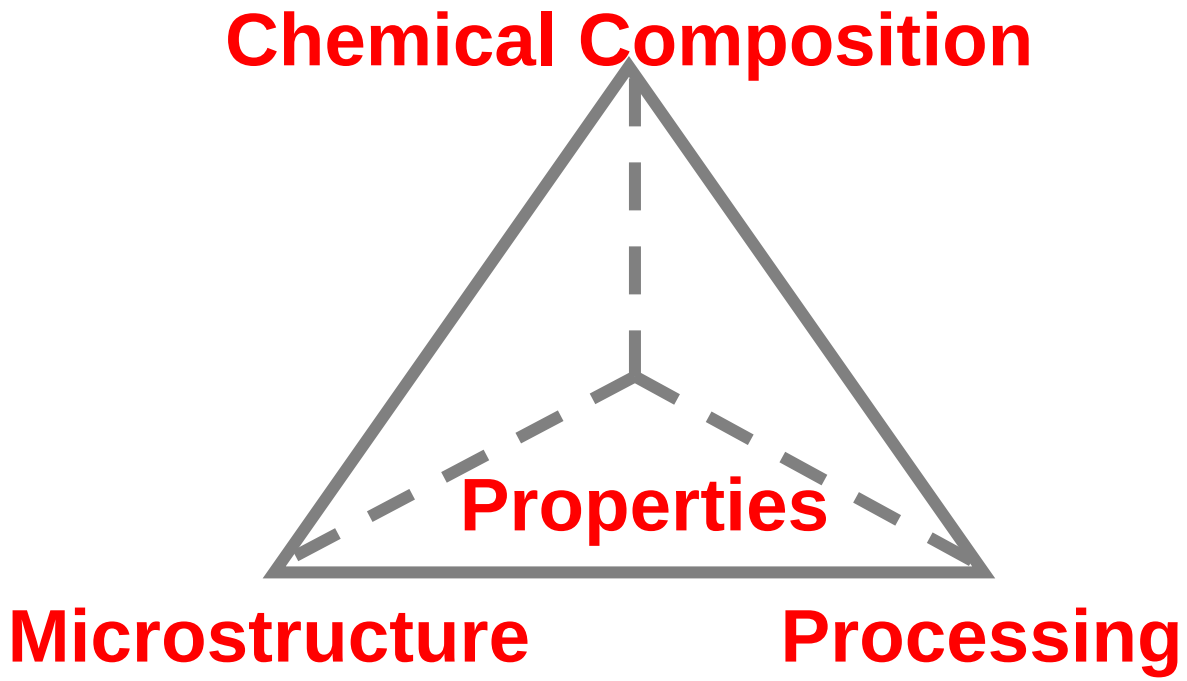
June 2011

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.

The influence of chemistry on microstructure and properties



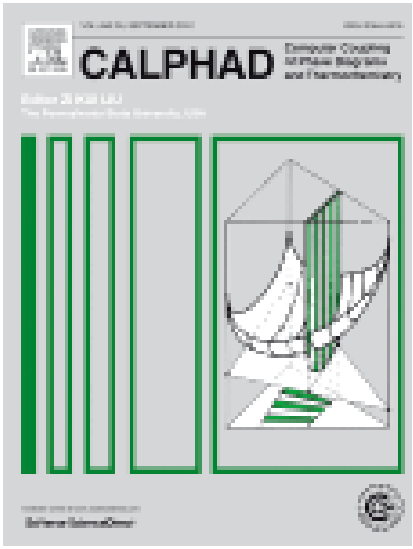
Heat treating can best be defined as "the controlled application of time, temperature and atmosphere to produce a predictable change in the internal structure (i.e. the microstructure) of a material." Dan Herring, 100th Column of the "Heat Treat Doctor" published in Industrial Heating magazine

What 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.

What is CALPHAD?

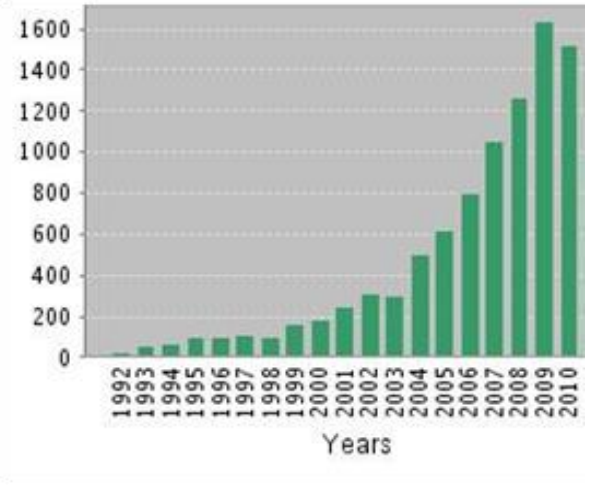
CALculation of PHAse Diagrams



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.

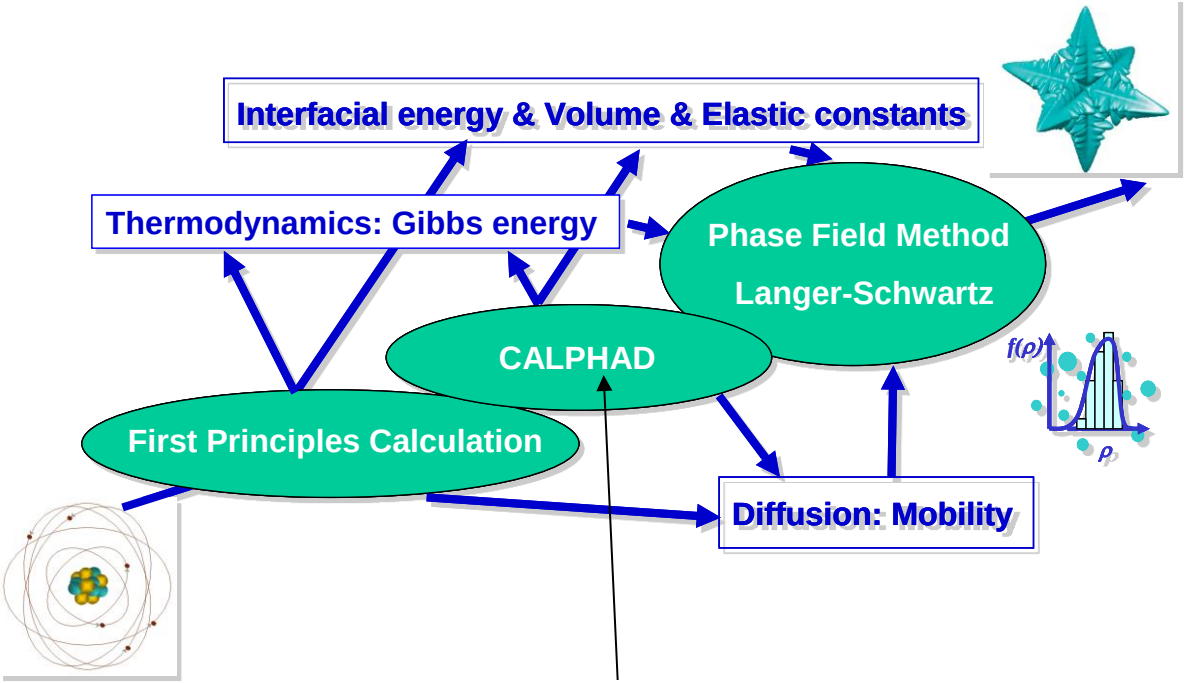
An international community, and conference held each year with 150-300 active participants from around the world.

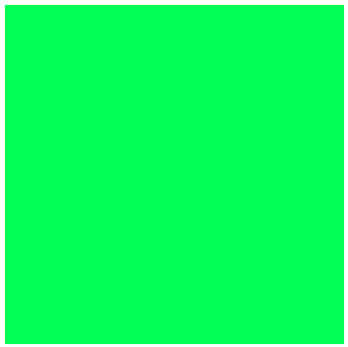


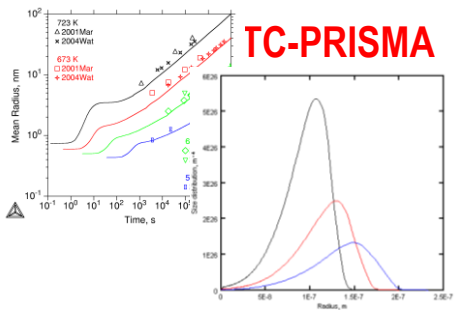
CALPHAD – an important bridge to multicomponent prediction

Towards prediction of microstructure evolution and material properties

Bridging Atoms and Microstructure

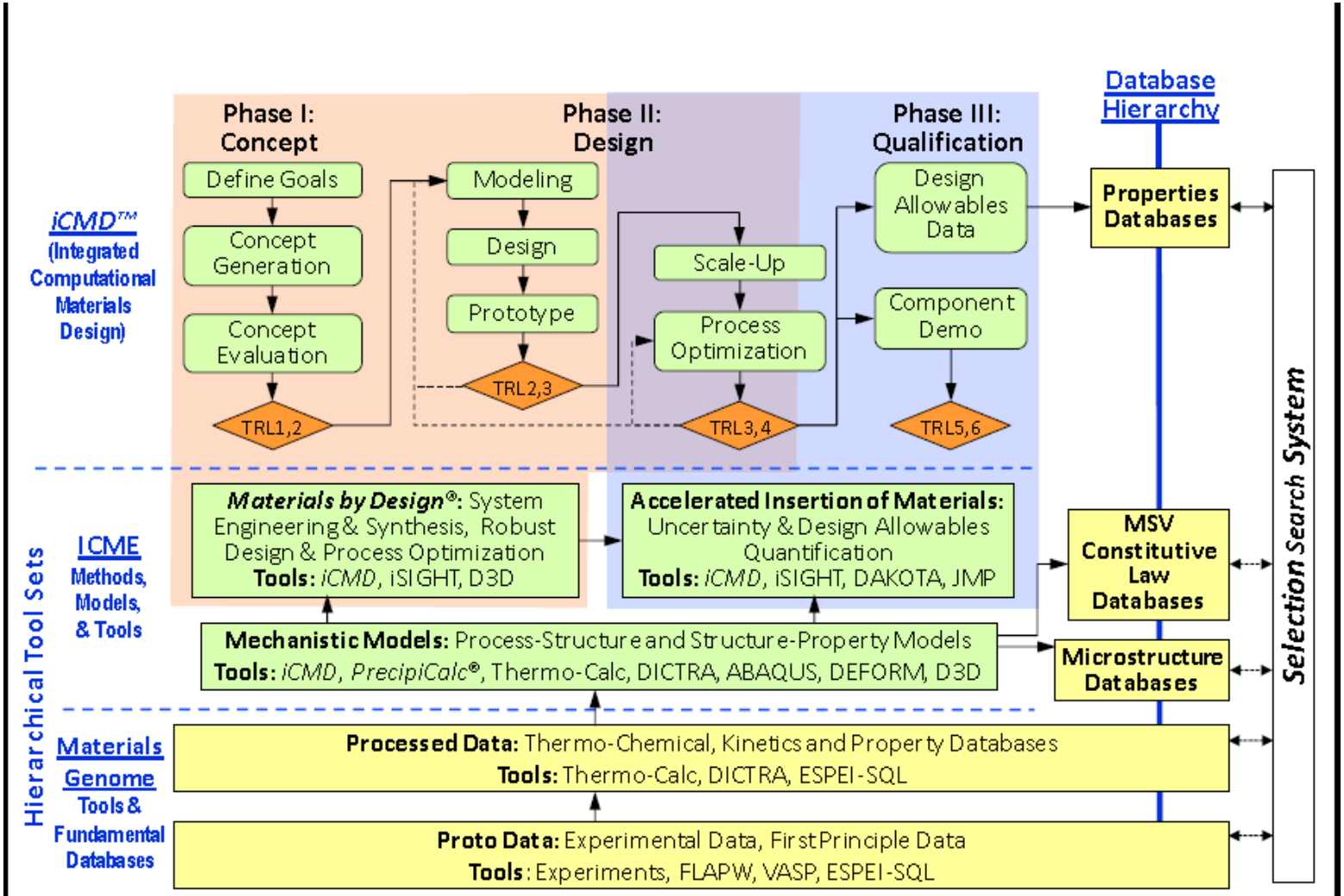






The development of consistent databases where each phase is described separately using models based on physical principles and parameters assessed from experimental data is a key.

CALPHAD – a foundation of MGI, ICME and ICMD



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

Requirements for modeling microstructure evolution

The phases that form and their composition under given conditions (over-all composition, temperature and pressure) *(Thermo-Calc)*

How do these quantities evolve in time? *(DICTRA, TC-PRISMA, phase field)*

- Synthesis and processing
- Usage

Length scale of microstructure *(Phase-field)*

Stresses

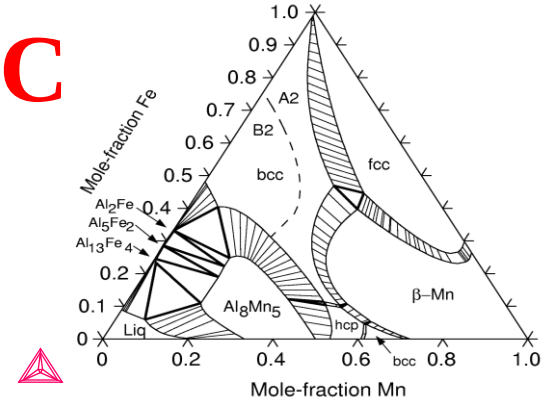
Details of morphology

Statistics – size distributions etc *(TC-PRISMA)*

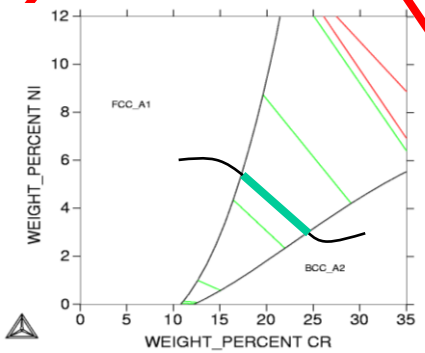
Slide courtesy of Prof. J. Ågren, KTH

A suite of CALPHAD based software tools

THERMO-CALC

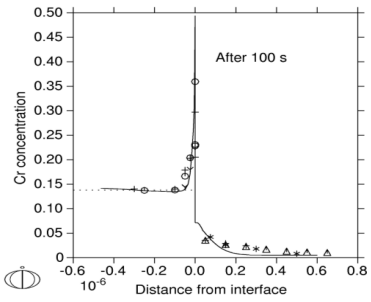


Driving forces



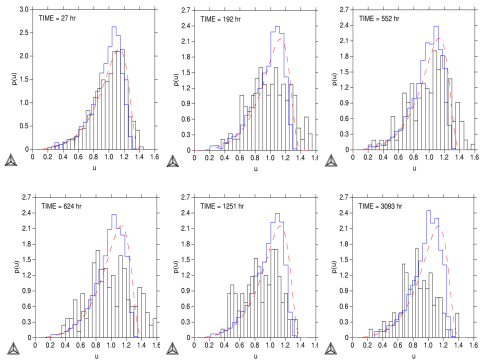
Interfacial energies

DICTRA

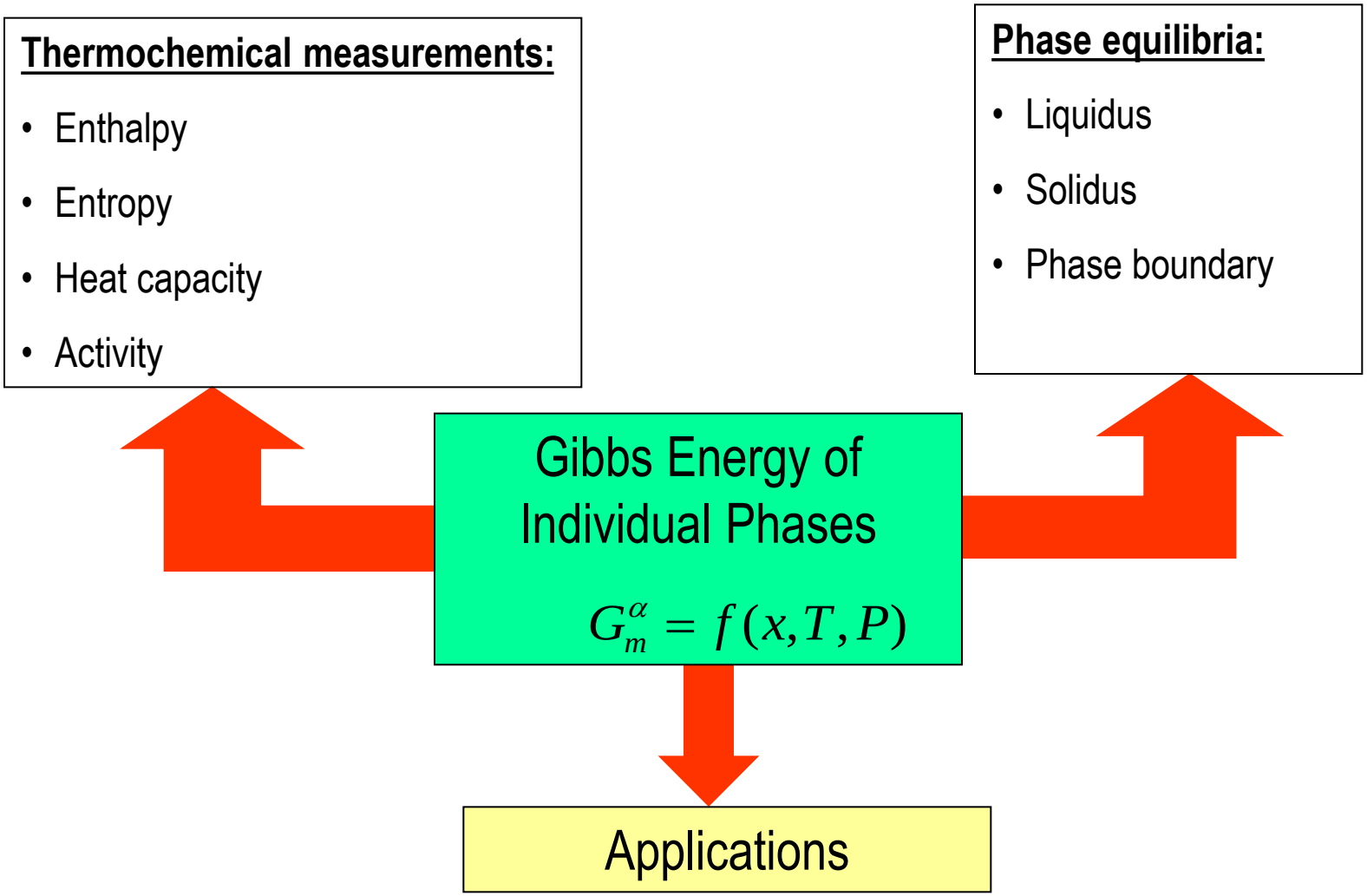


Diffusivities

TC-PRISMA



What is CALPHAD (1)



What is CALPHAD (2)

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

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

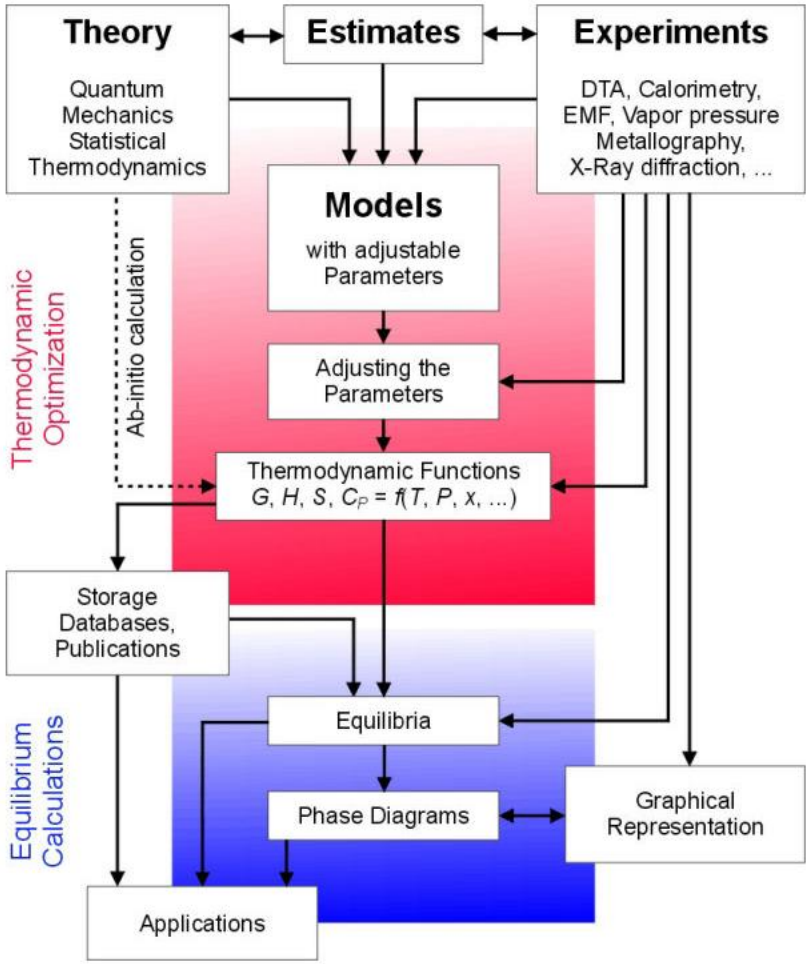
reference surface

configurational contribution

excess term

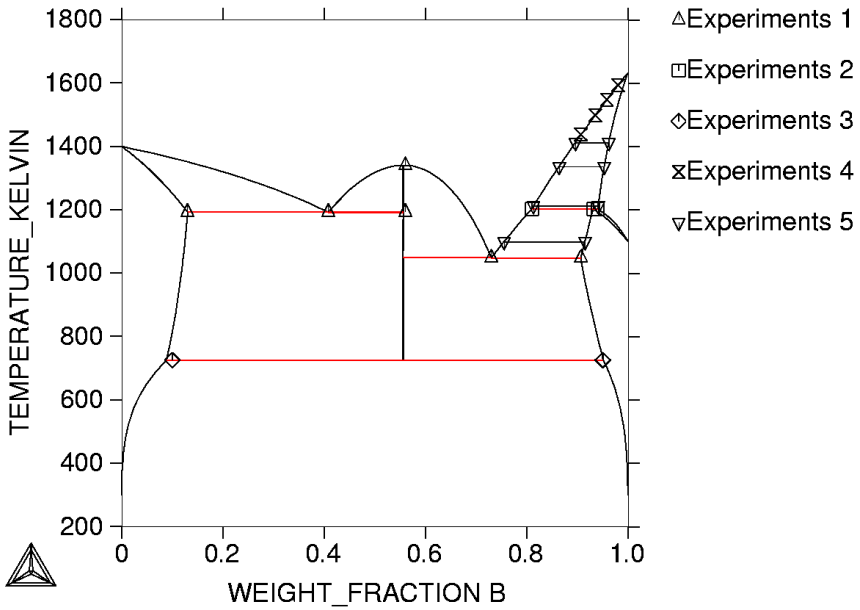
physical contribution

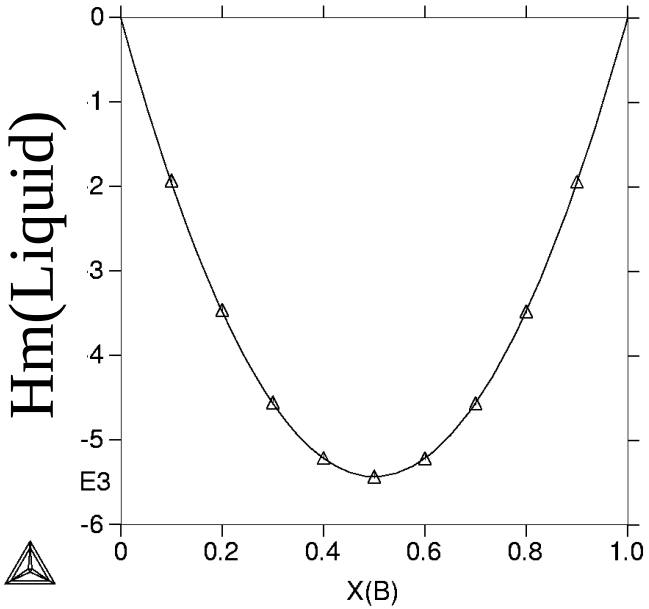
What is CALPHAD (3)



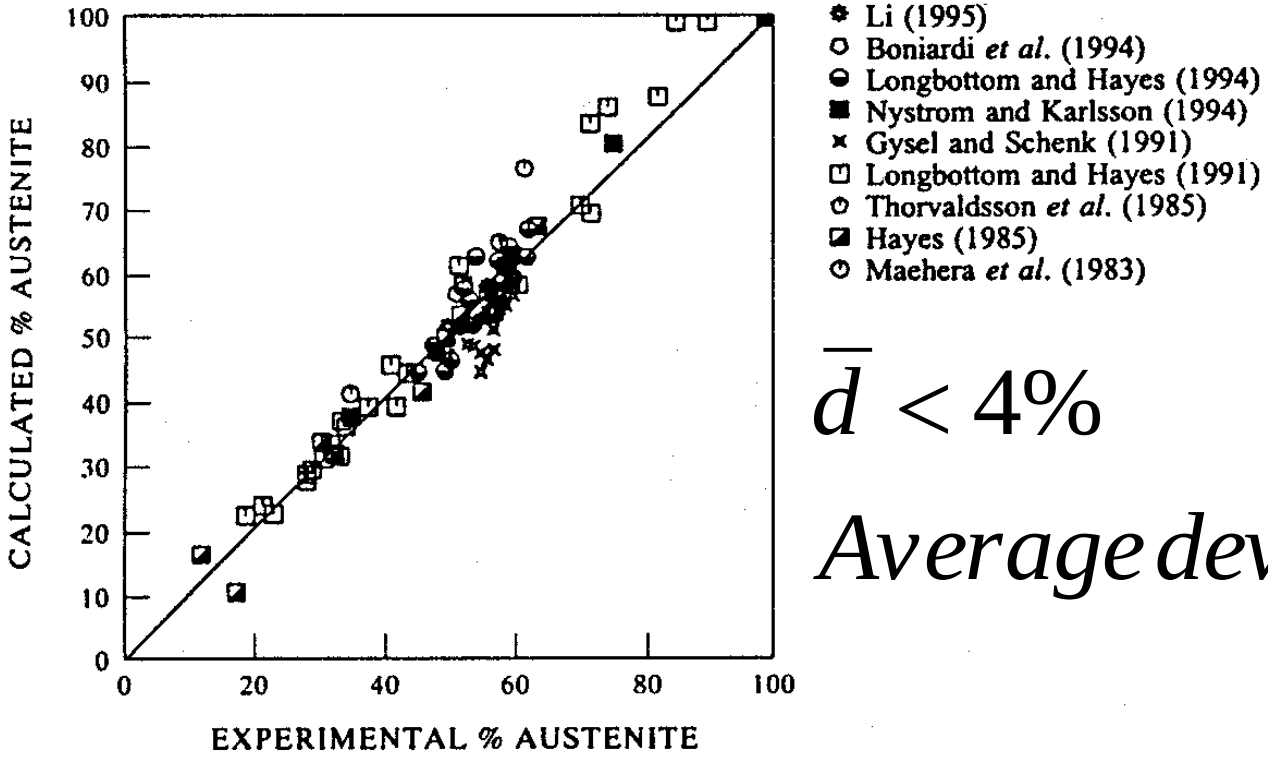
What is CALPHAD (4)

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





What is CALPHAD (5)



$\bar{d} < 4\%$

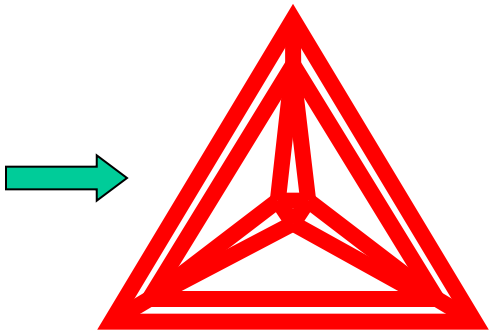
Average deviation

Figure 10.40 Comparison between calculated and experimentally observed % of austenite in duplex stainless steels. (Data from Longbottom and Hayes (1991) represent dual phase steels.).

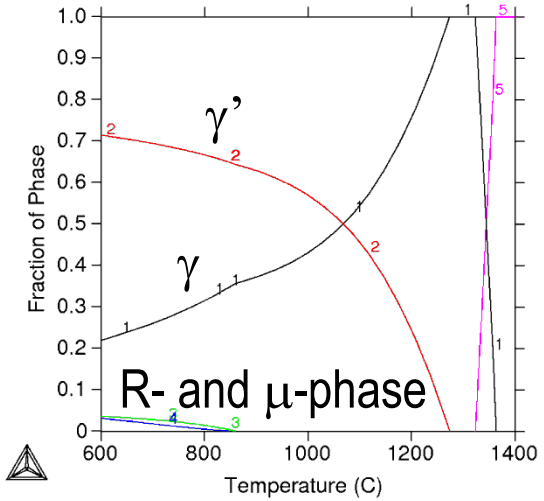
From: Saunders & Miedownik: "Calphad -a comprehensive review"

What is CALPHAD (6)

Thermodynamic Database



Thermo-Calc



Description of Gibbs free energy for the individual phases

$$G_m^{\phi}\left(T,P,x_i^{\phi}\right)$$

Minimization of the total Gibbs free energy under given conditions.

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

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

Result

Thermodynamic databases

A wide range of thermodynamic databases are available for:

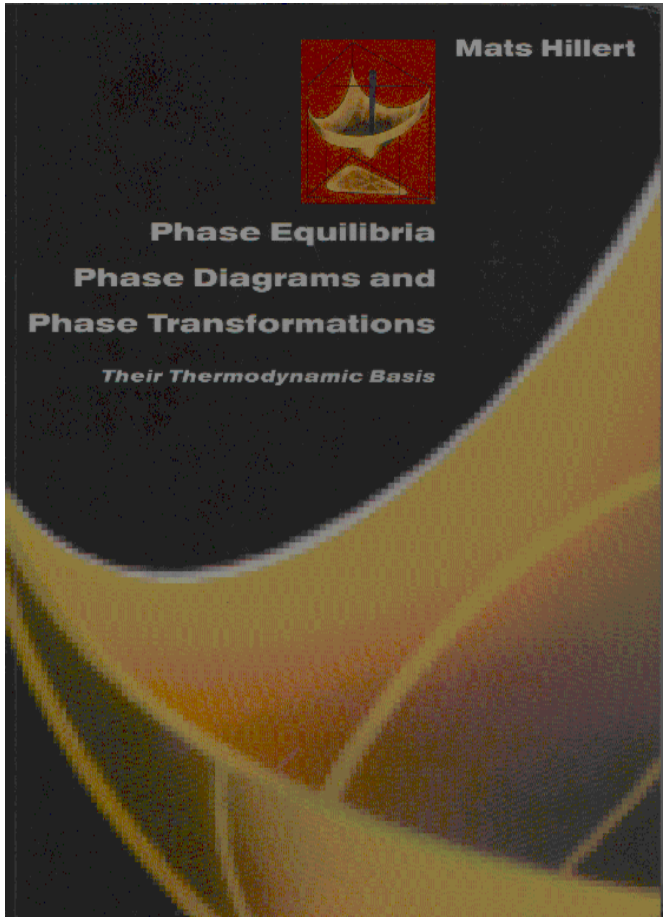
- Steels and Fe-alloys
- Nickel-base superalloys
- Aluminium/Titanium/Magnesium-base alloys
- Gases, pure inorganic/organic substances, & general alloys
- Slag, metallic liquids, and molten salts
- Ceramic systems, and hard materials
- Semiconductors, and solder alloys
- Noble metal alloys
- Materials 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

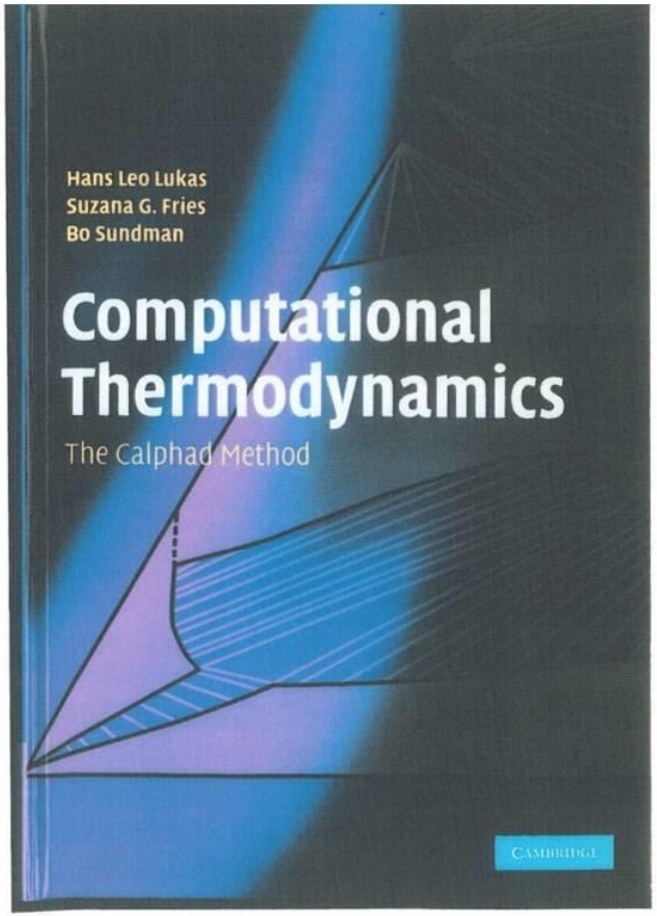
	Al	B	C	Co	Cr	Fe	Hf	Mo	N	Nb	Ni	Pd	Pt	Re	Si	Ta	Ti	V	W
B	x																		
C	x	x																	
Co	x	x	x																
Cr	x	x	x	x															
Fe	x	x	x	x	x														
Hf	x	x	x	x	x	x													
Mo	x	x	x	x	x	x	x												
N	x	x		x	x	x		x											
Nb	x	x	x	x	x	x	x	x	x										
Ni	x	x	x	x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

CALPHAD – additional references



ISBN 978-0-521-85351-4



ISBN 978-0-521-86811

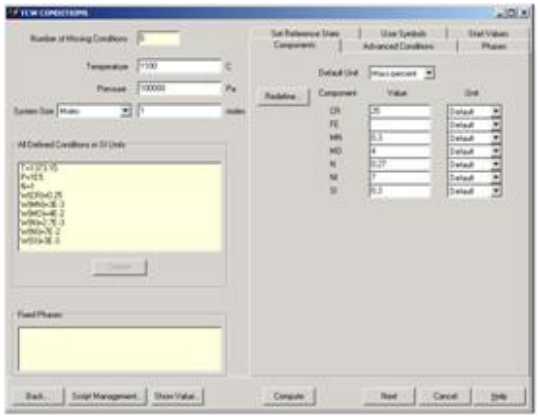
CALPHAD based software: Thermo-Calc (1)

- 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….**

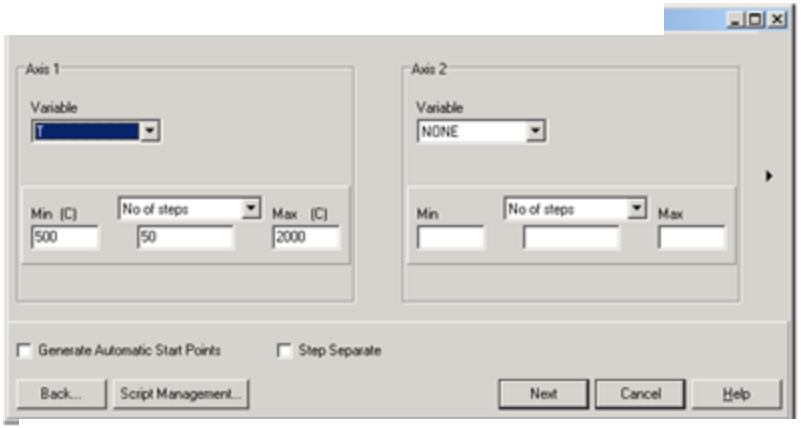
- Designing and optimization of alloys
- Design and optimization of processes

CALPHAD based software: Thermo-Calc (2)

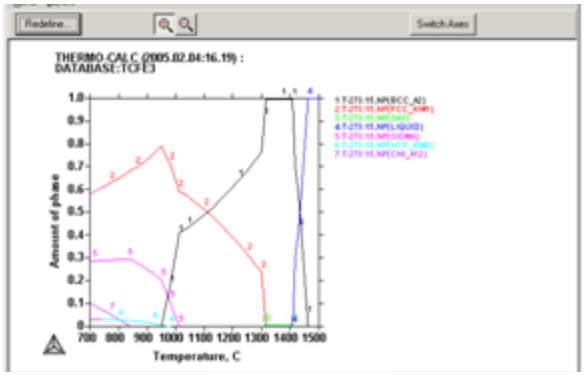
1. Define your system
TCW Material



2. Set your input conditions
TCW Conditions



3. Set calculation variables.
TCW Map/Step Definition



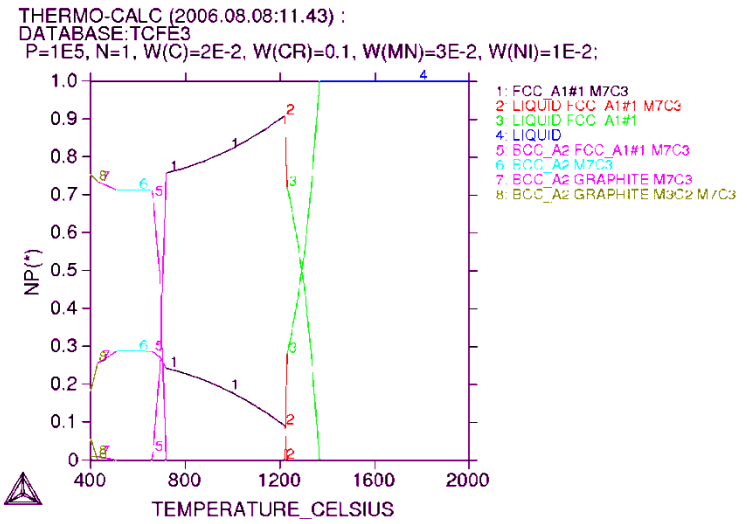
4. Plot your output
TCW Diagram Definition

CALPHAD based software: Thermo-Calc (3)

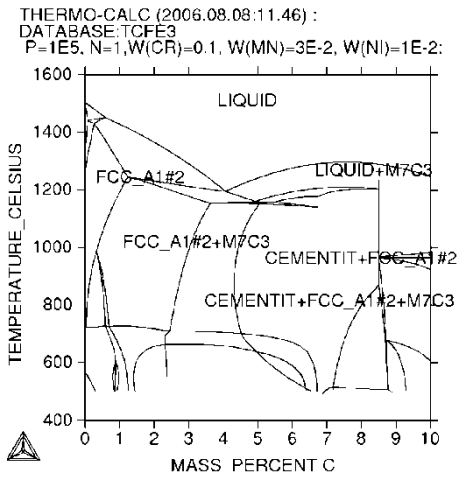
Single Pt Eqm

```
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
```

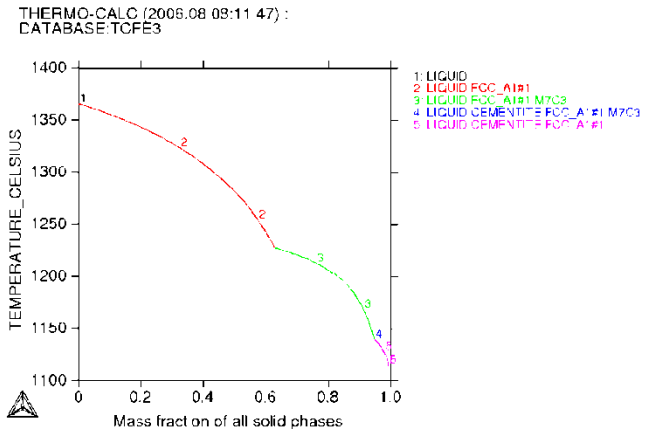
STEP



MAP



SCHEIL



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

CALPHAD based software: DICTRA

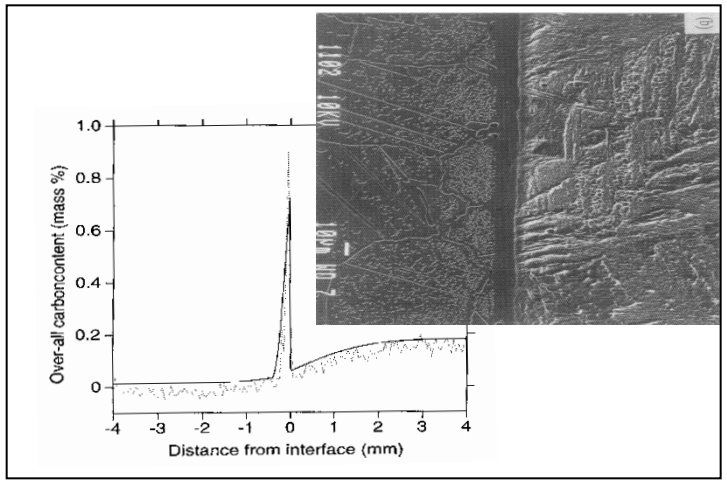
•A general software package for simulation of **DI**ffusion **C**ontrolled **TRA**nsformations in multi component alloys.

•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



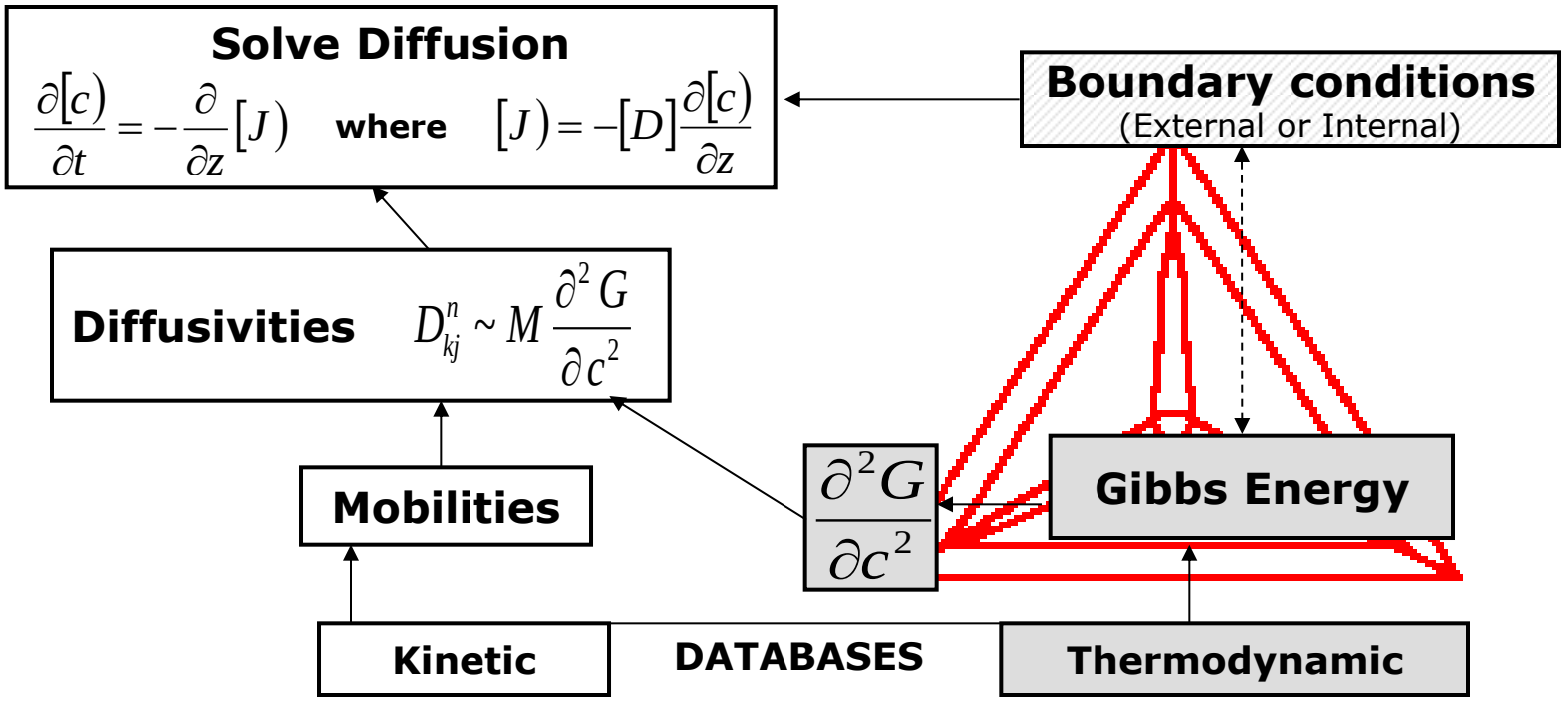
Emphasis has been placed on linking fundamental methods to critically assessed thermodynamic and kinetic data, allowing simulations and predictions to be performed with realistic conditions on alloys of practical importance.

Helander et al., ISIJ Int. ***37****(1997), pp. 1139-45*

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

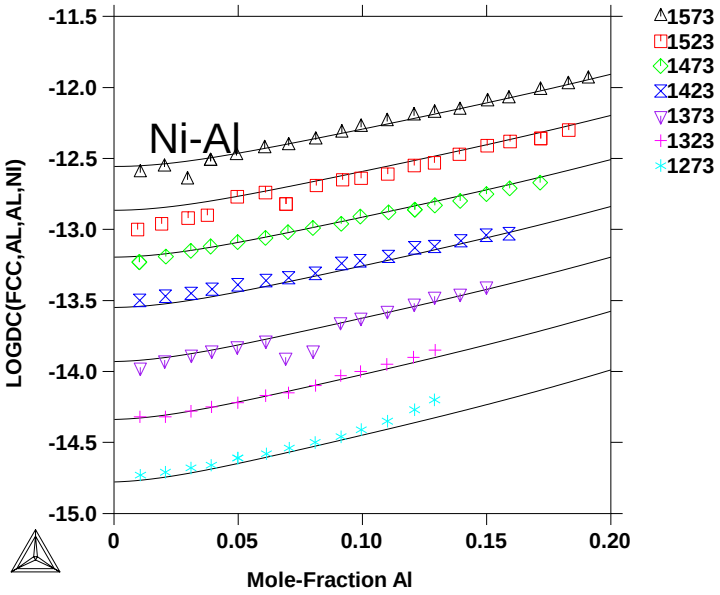
- Modelling must apply in multicomponent systems because the real alloys are multicomponent. Many diffusion coefficients!
- Various type of coupling effects may make it more complicated than Fick's law.
- Details of geometry not of primary importance.
- An approach in the Calphad spirit was suggested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

Slide courtesy of Prof. J. Ågren, KTH

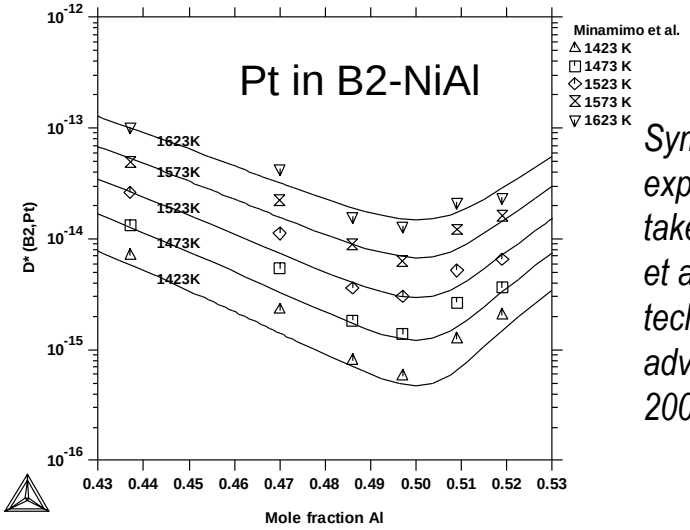
Available Kinetic Databases

Mobility databases are currently available for:

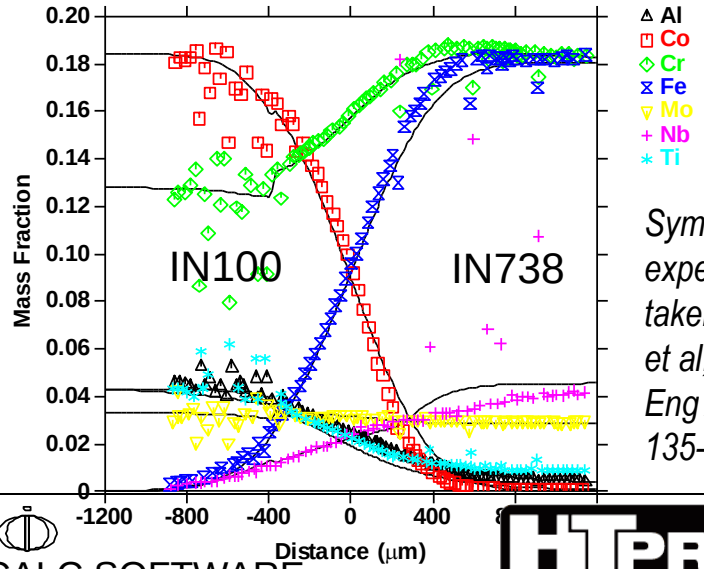
- Steels and Fe-alloys
- Nickel-base superalloys
- Aluminium alloys



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.



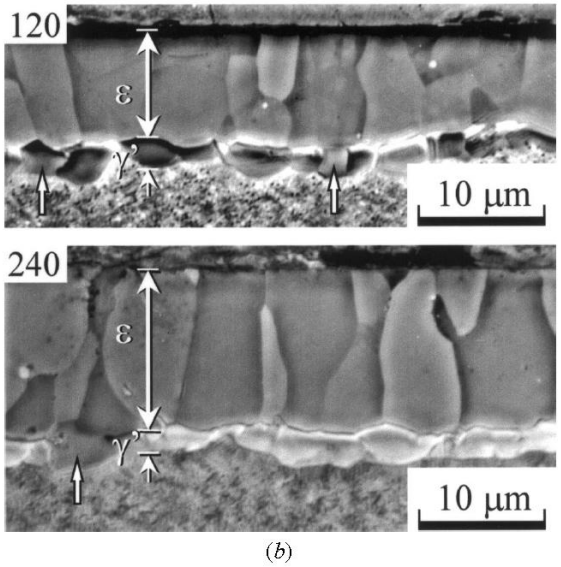
Symbols are experimental data taken from Campbell et al, Materials Sci & Eng A ***407****(2005), pp. 135-146.*

Example of thermodynamics + diffusion - Nitriding

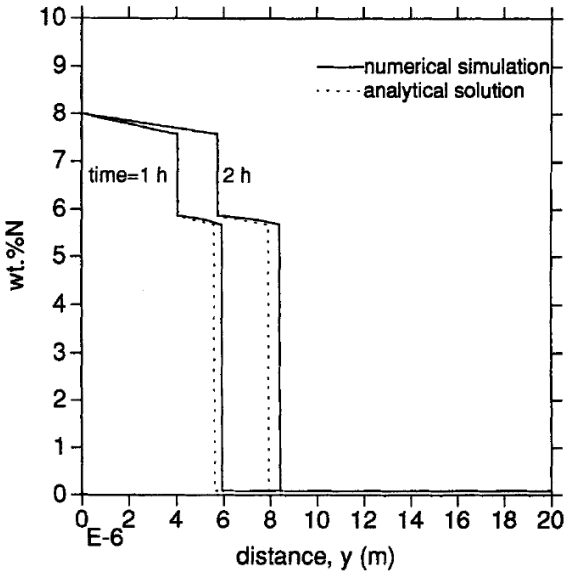
– Nitride formation at steel surface during nitriding of steel:

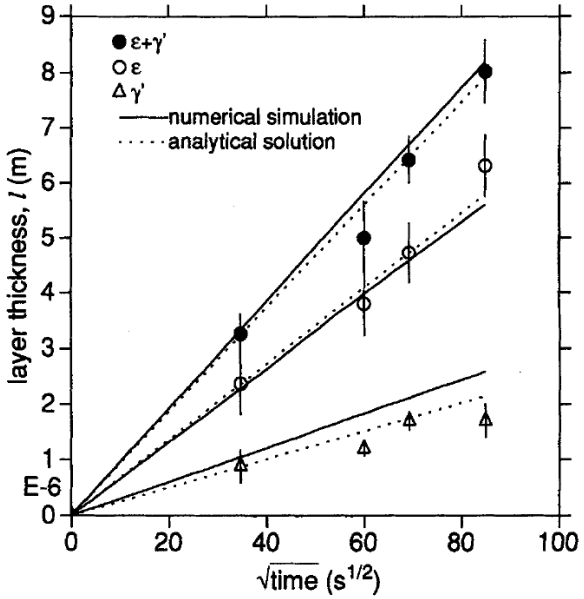
(Du et al. 1996, 1998)

- A surface modification process with many advantages. How thick are the surface layers?



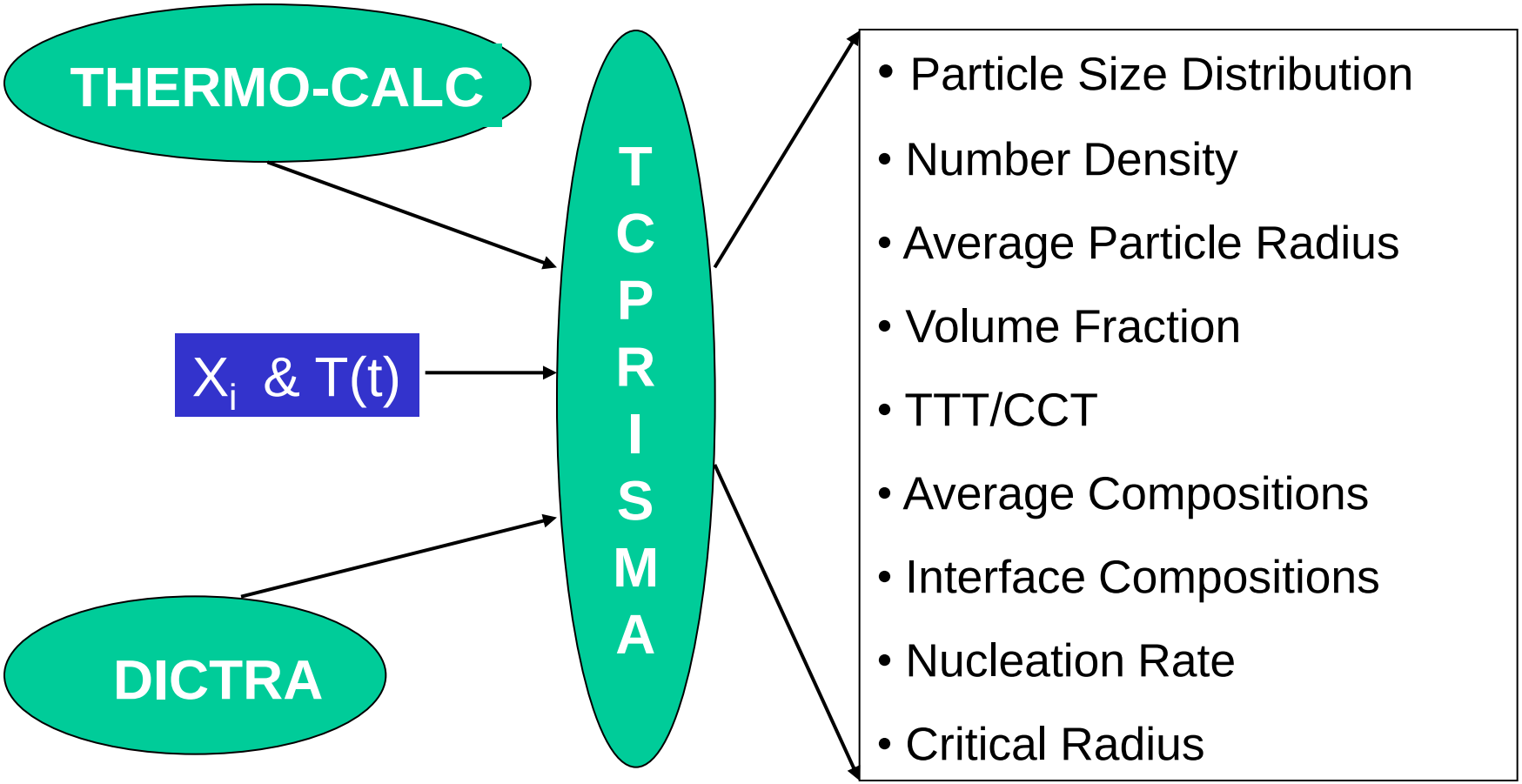
(b)





CALPHAD based software: TC-PRISMA (1)

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



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.

CALPHAD based software: TC-PRISMA (2)

Classic Nucleation Theory

Grain size, dislocation density, etc

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

Interfacial energy Volume

$$Z = \left\{\frac{-1}{2\pi kT}\left(\frac{\partial^2 \Delta G_n}{\partial n^2}\right)_{n^*}\right\}^{1/2} \qquad \Delta G^* = \frac{16\pi\sigma^3 V_m^2}{3\Delta G_m^2}$$

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

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

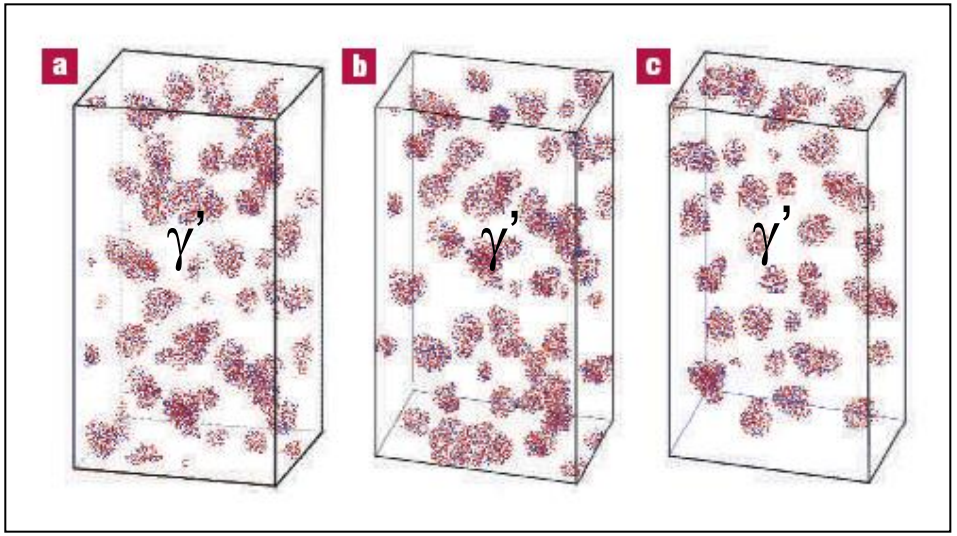
Ni-9.7Al-8.5Cr-2W

Ni-7.5Al-8.5Cr

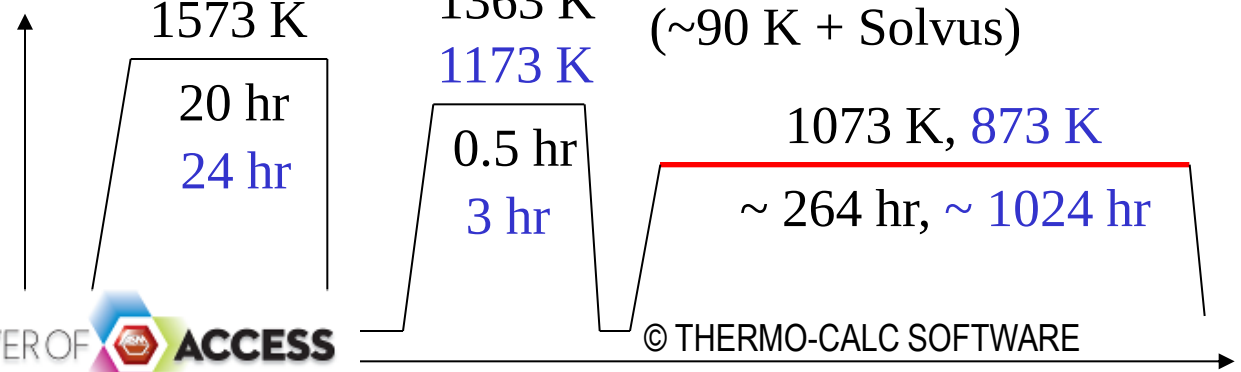
Ni-5.2Al-14.2Cr

$\sigma = 0.023$ J/m^2

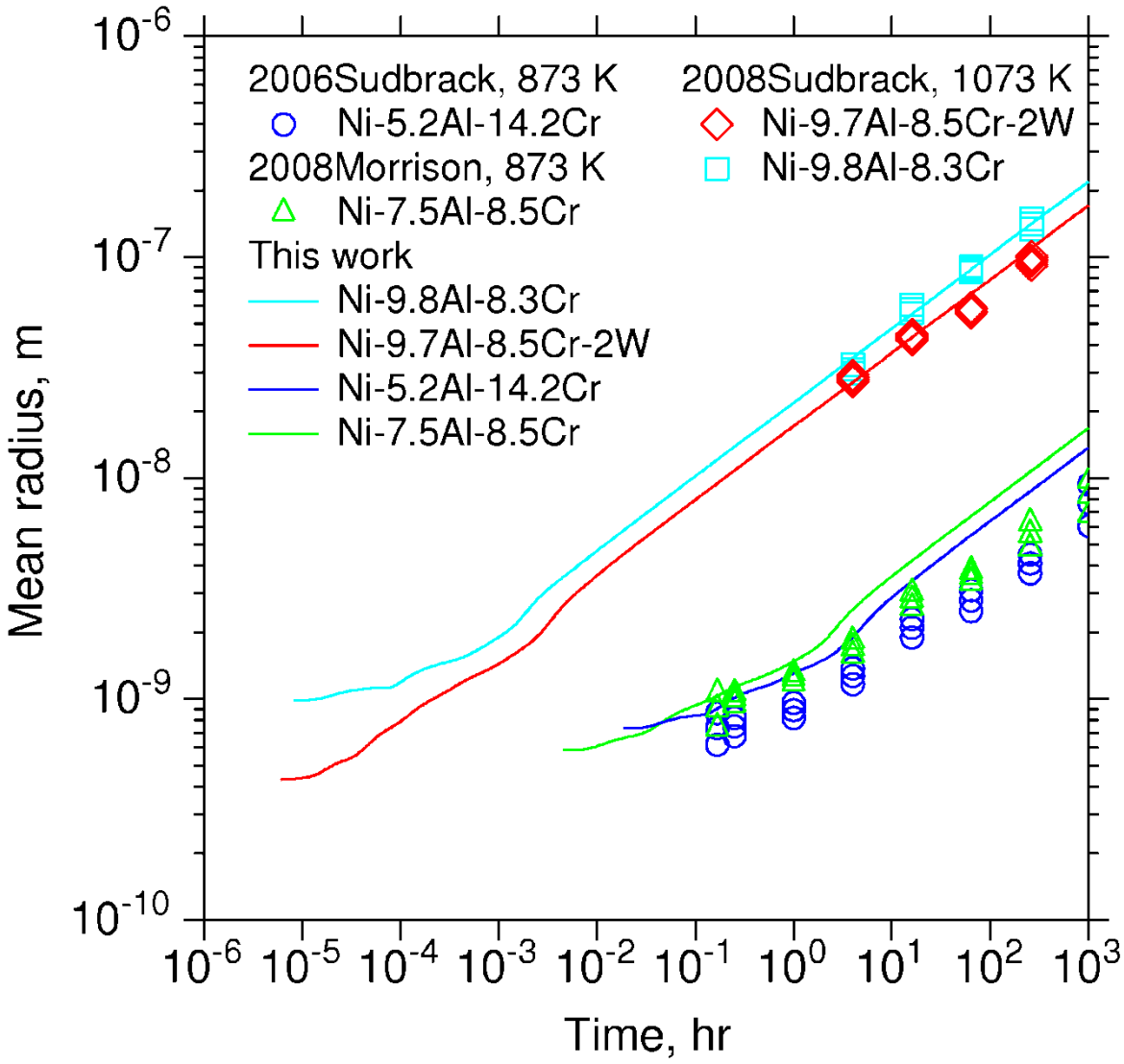
Thermo-Calc and Dictra Databases



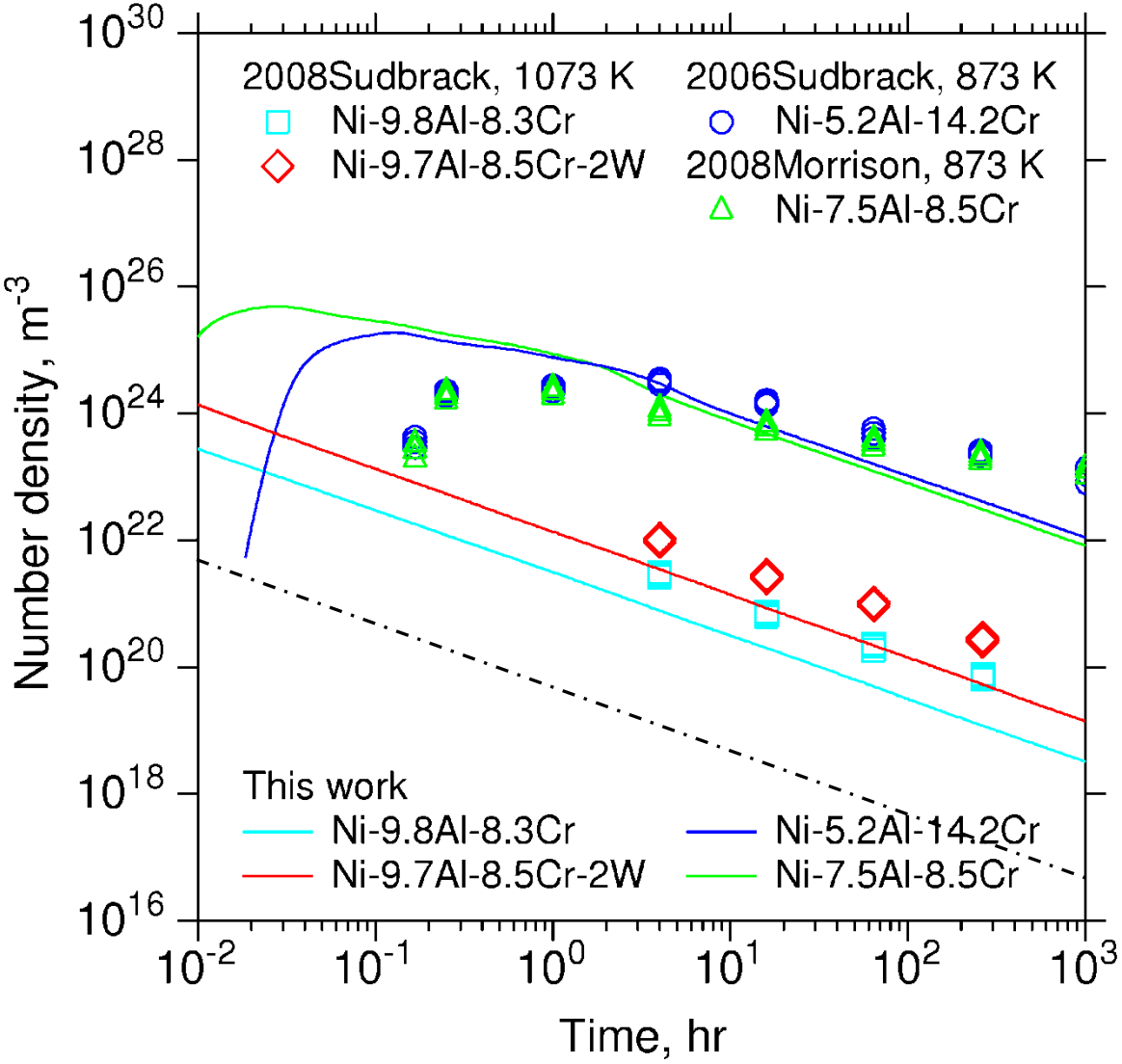
Mao et al, Nature materials, 6(2007)210-216



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

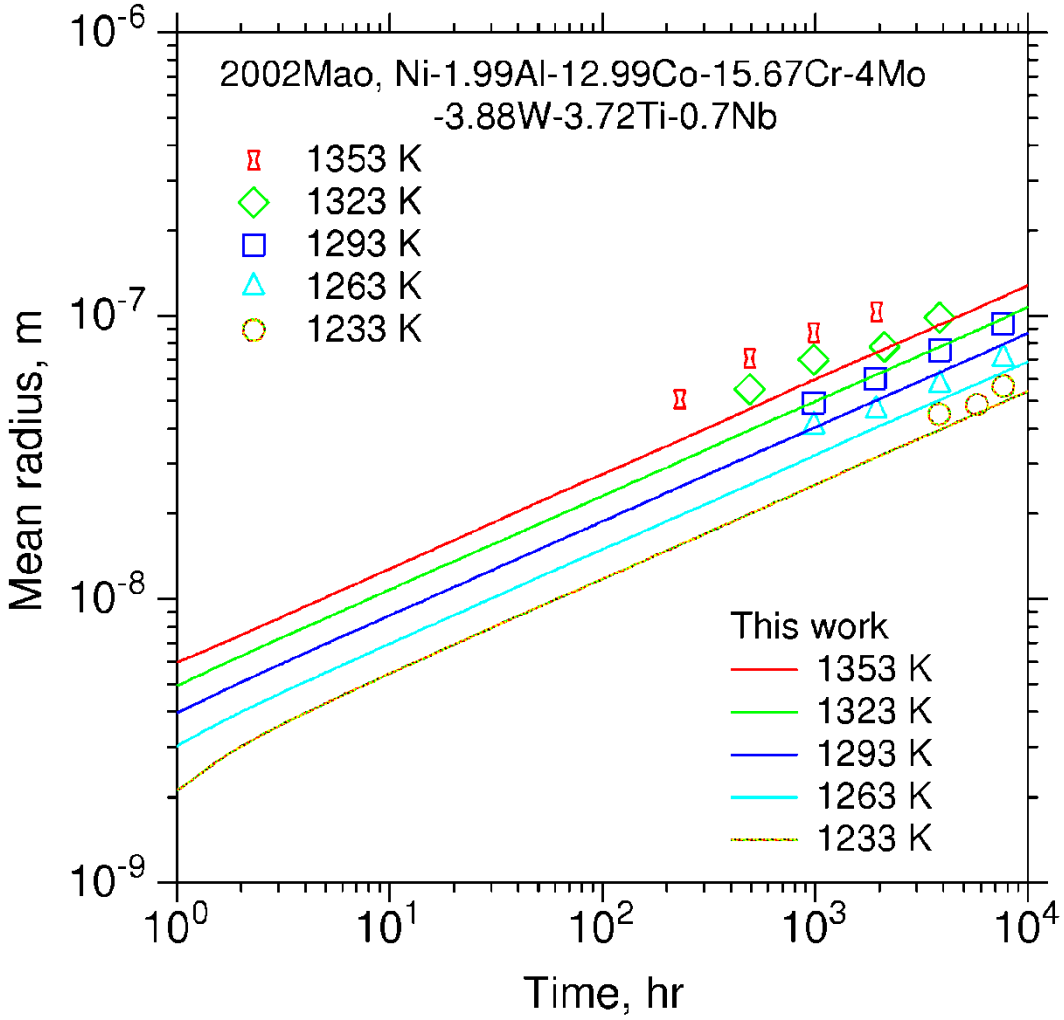


TC-PRISMA Examples: Ni-based superalloy (3) – Number density

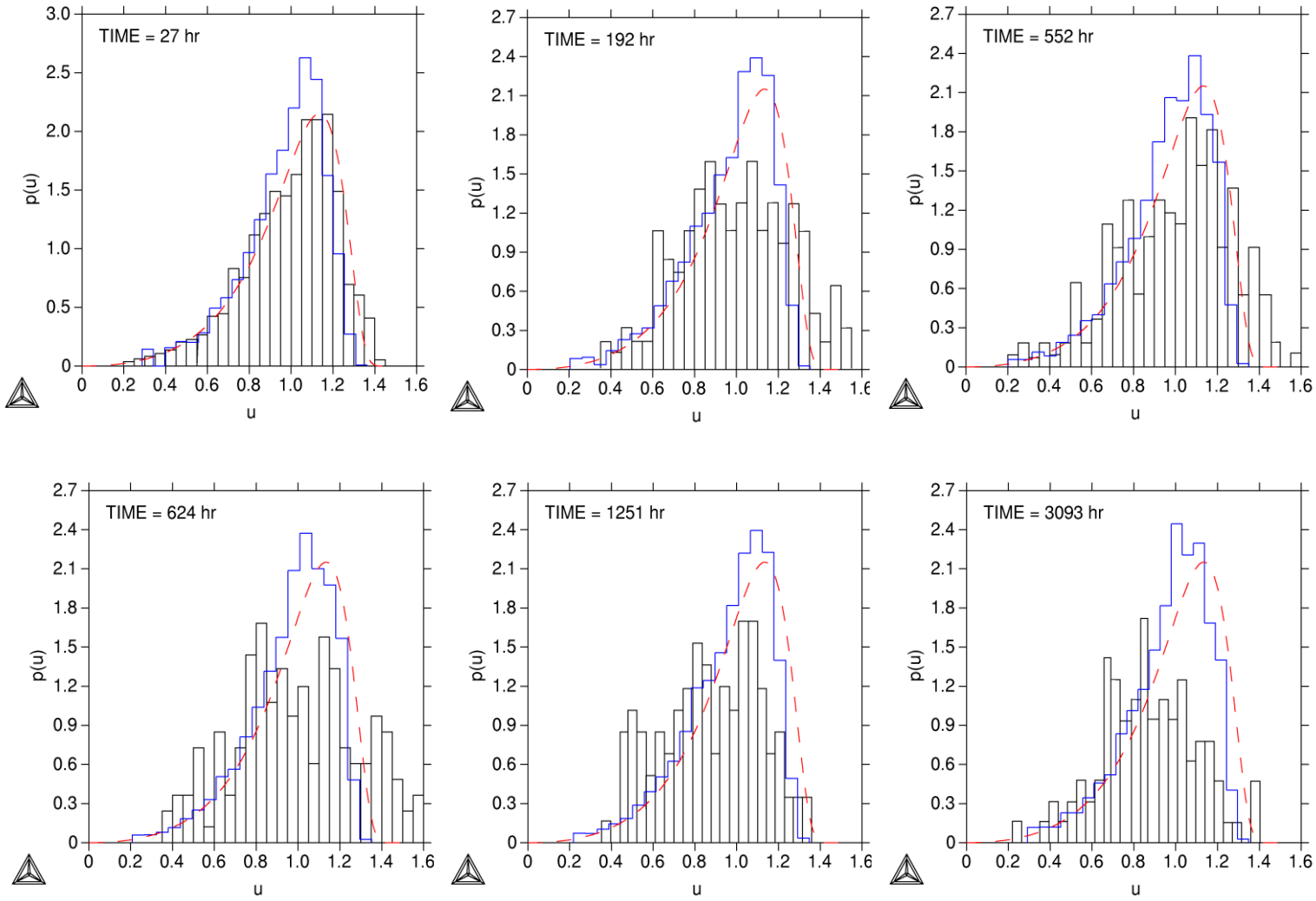


TC-PRISMA Examples: Ni-based superalloy (4) - Rene88DT

Change only system and use same set of physical parameters



TC-PRISMA Examples: Particle size distribution



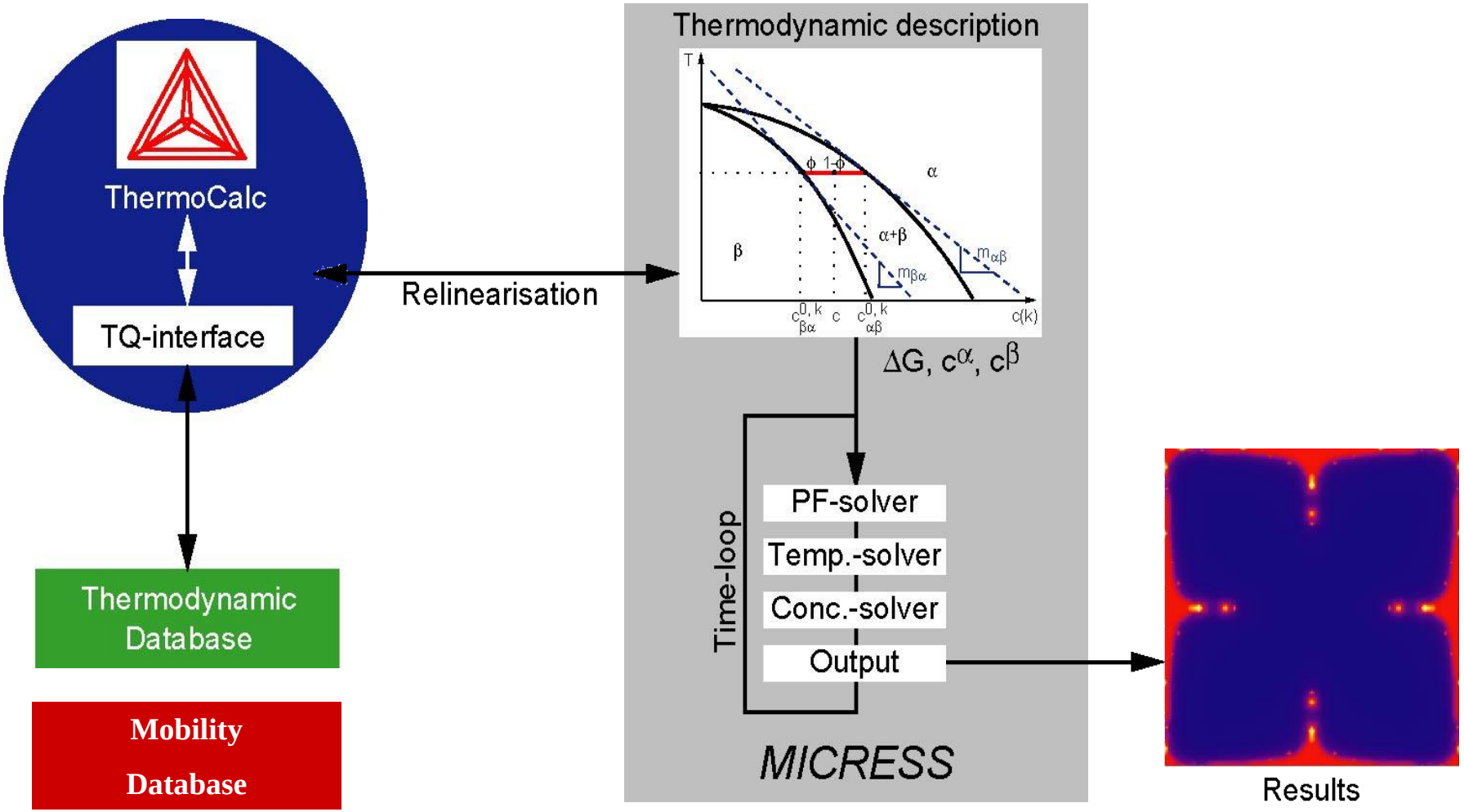
CALPHAD based software: Phase field (1)

- 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



Examples with application to the materials life cycle

R&D - alloy design

Metallurgical extraction

Casting

Forging/Rolling

Heat-treatment

Joining/
Welding

Quality control

Materials selection

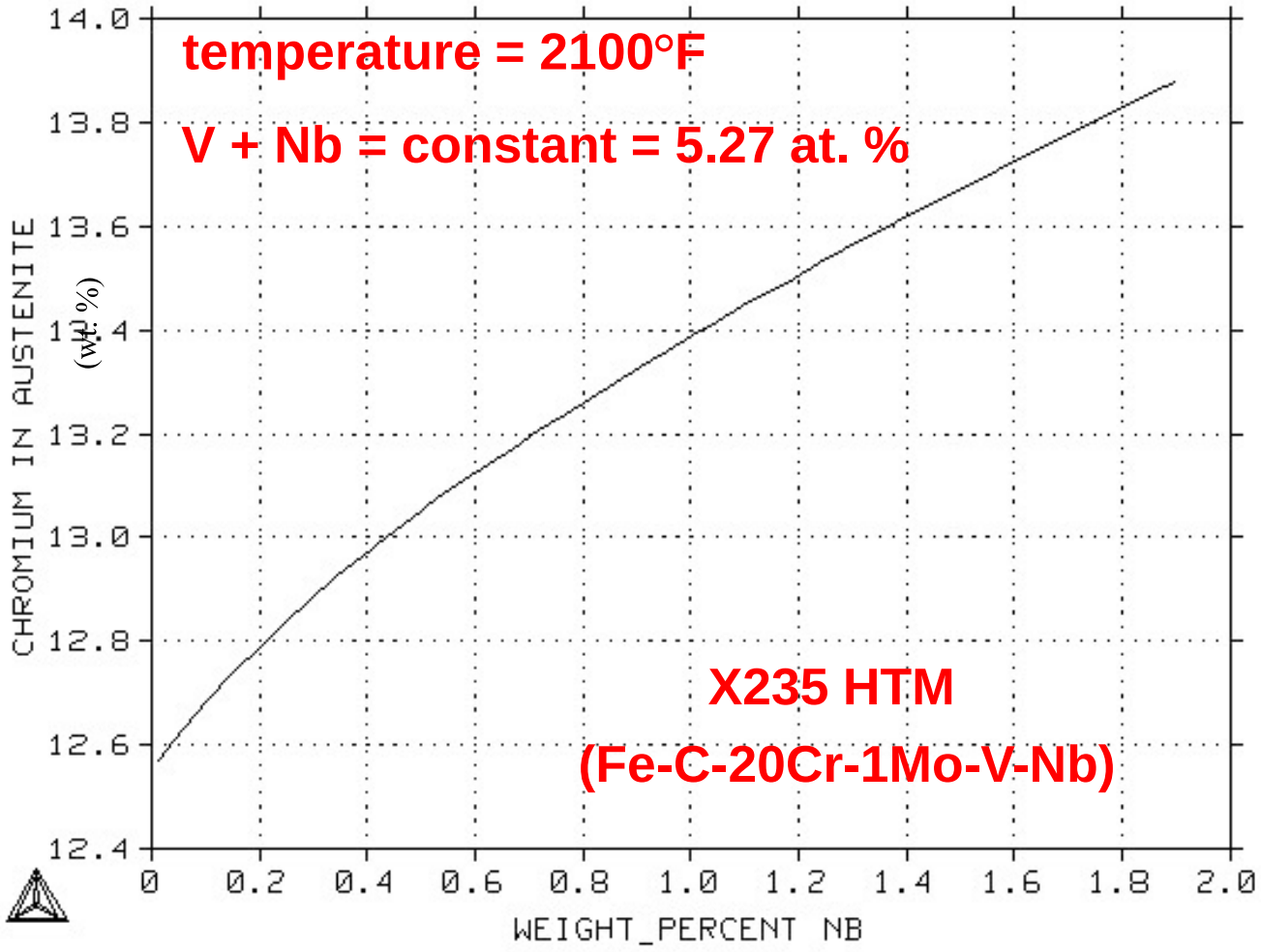
Corrosion

Failure analysis

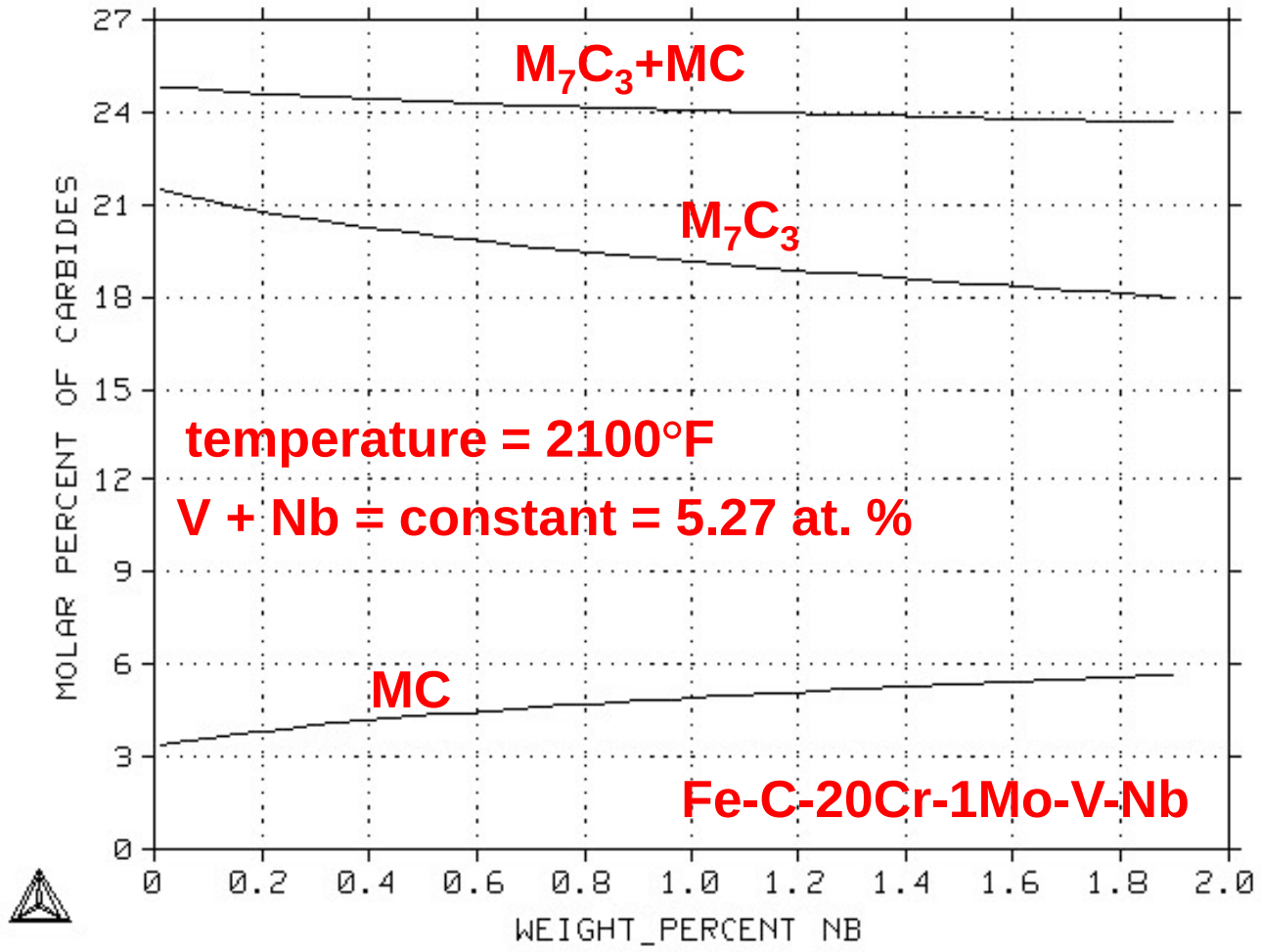
Waste and re-cycling

Example: Influence of alloy composition (1)

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



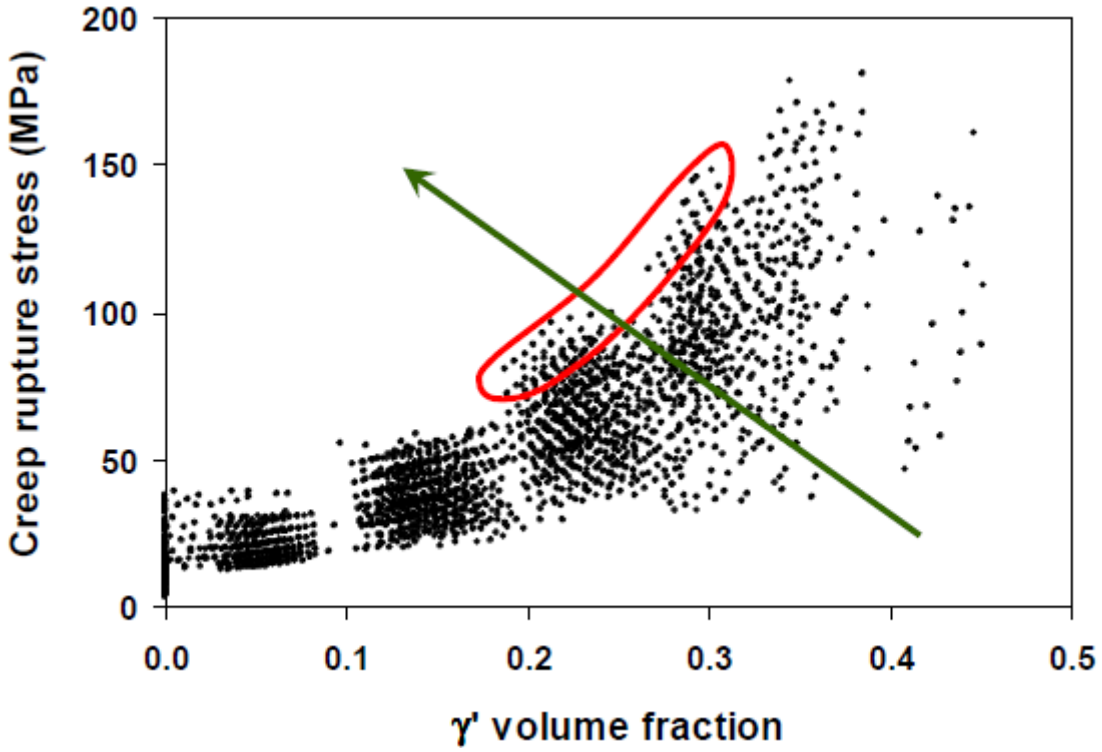
Example: Influence of alloy composition (2)



Example: Optimization of an alloy composition

Franck Tancret – Université de Nantes (TMS 2009):

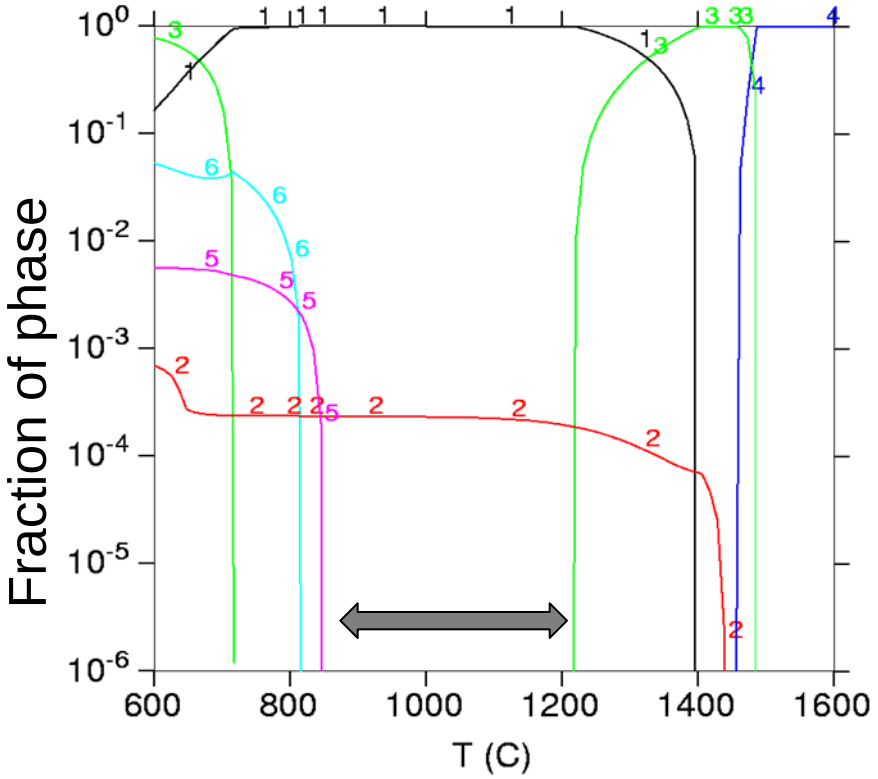
Optimization of an alloy composition for the design of weldable and creep resistant superalloys using Matlab, TC-Matlab toolbox and neural net models. Over 16,000 compositions assessed.

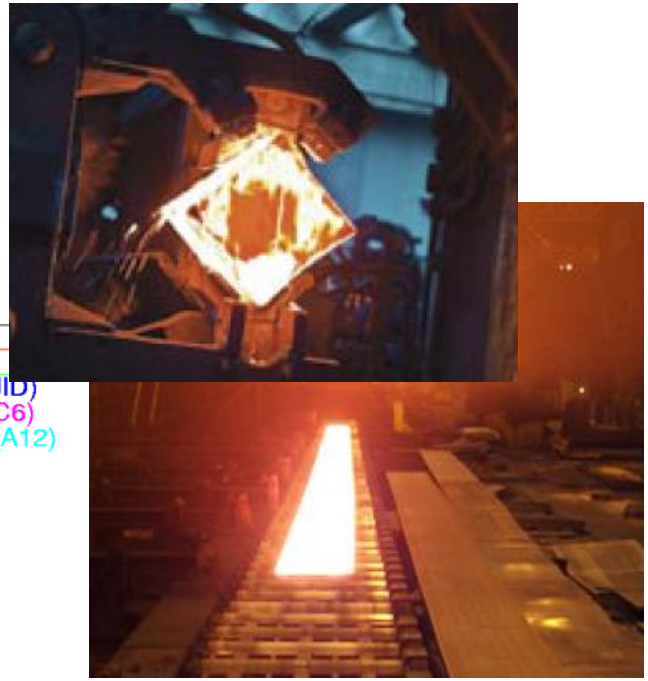


Example: Forging and hot rolling

- Selecting optimum temperature for operation.

  Safe forging of supermartensitic stainless in γ-field





C 0,02%
Cr 12%
Ni 5%
Mo 2%
Mn, Si
Ti, N,

Courtesy André

Example: Homogenizing a Ni based superalloy (1)

Homogenizing a Nickel based superalloy: Thermodynamic and kinetic simulation and experimental results.
Paul D Jablonski and Christopher J Cowen (NETL, Albany, OR)
Met. Trans. B. Vol 40B, April 2009 (pp 182-186)

Table I. Target and Measured Chemistry (in Weight Percent) of the Nimonic 105 Alloy Cast for This Study

Nimonic 105	C	Cr	Mo	Co	Al	Ti	Mn	Si	B
Target	0.15	14.85	5	20	4.7	1.1	0.5	0.5	0.05
Measured	0.16	14.61	5.02	20.04	4.43	1.1	0.51	0.51	0.05

Example: Homogenizing a Ni based superalloy (2)

Thermodynamic data from the Thermotech Ni-data database
Mobility data from the MOBNi1 database.

Scheil calculation
used to predict the fraction solid curve and incipient melting temp -1142°C.

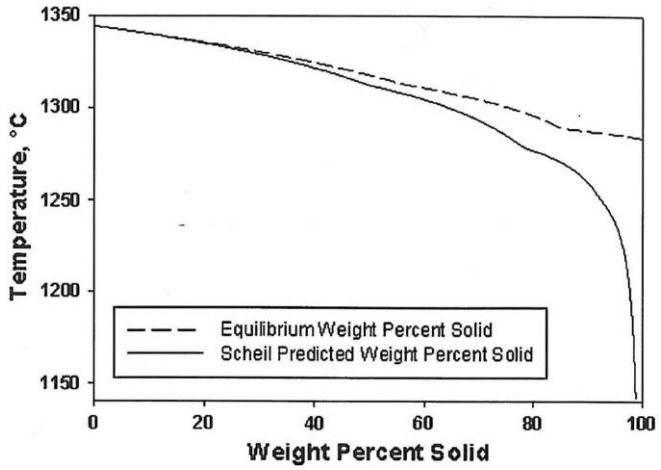


Fig. 1—Equilibrium and Scheil predicted solidification ranges for the Nimonic 105 alloy.

and extent of chemical microsegregation - amounts of each alloying element in the FCC (γ) phase

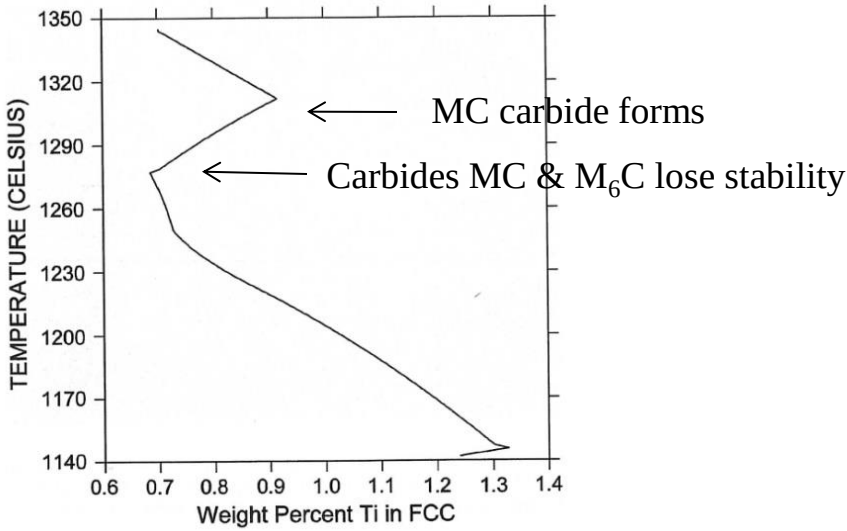


Fig. 2—Calculated amount of Ti in the fcc phase as a function of temperature.

Example: Homogenizing a Ni based superalloy (3)

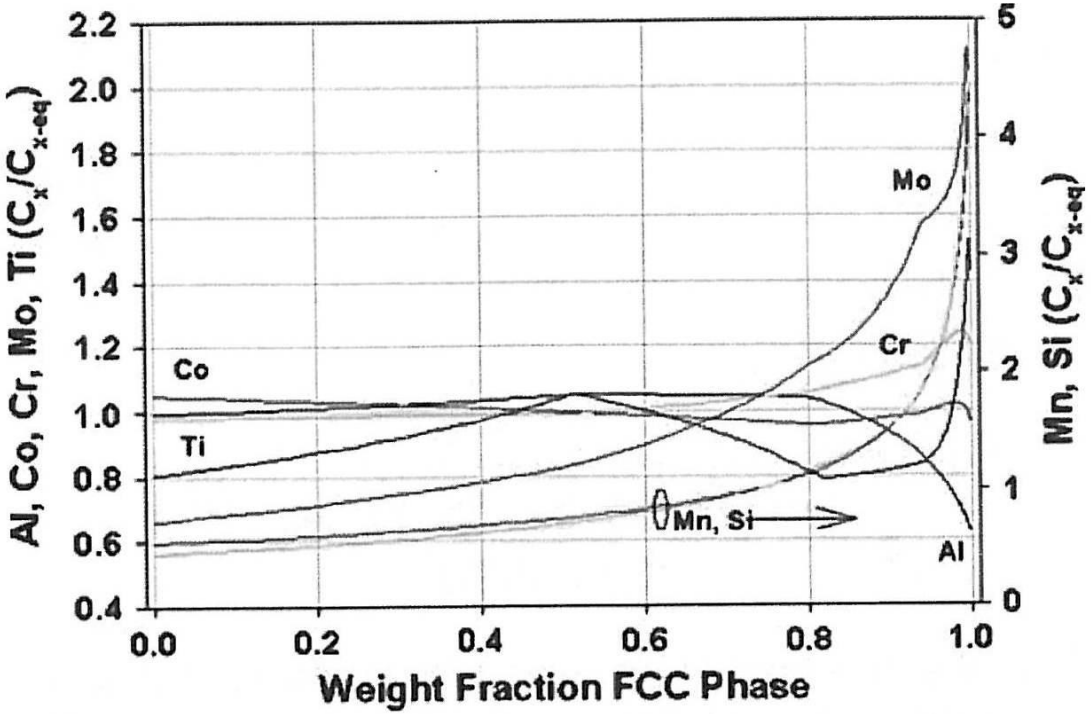


Fig. 3—Normalized Scheil predicted segregation across a dendrite (from center to edge).

Example: Homogenizing a Ni based superalloy (4)

DICTRA simulations performed to simulate homogenization.
Assumptions: Diffusion distance of 50 μm based on approx one half of the maximum secondary dendrite arm spacing. Weight fraction of FCC scaled to this distance and read into DICTRA along with the chemistry profiles across the FCC dendrites from the Scheil simulations.

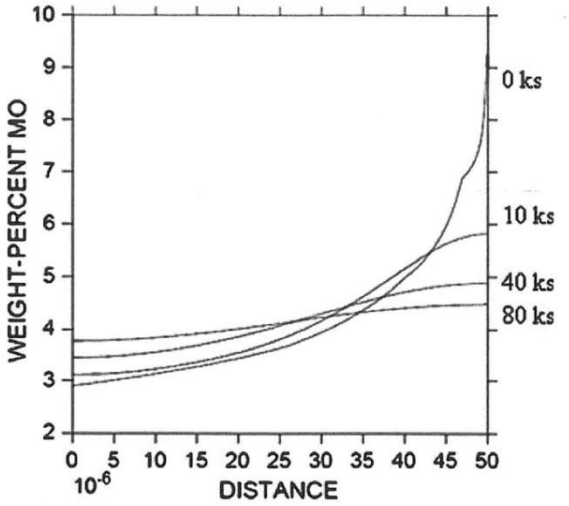


Fig. 4—Weight percent Mo as a function of distance (m) across a dendrite (from center to edge) for the following time sequences at 1100 °C: 0, 10, 40, and 80 ks.

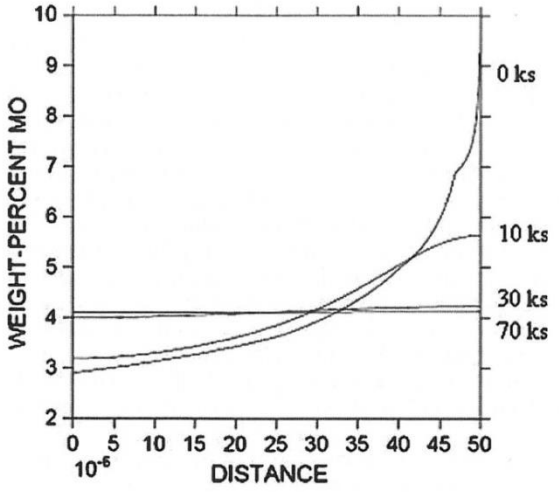


Fig. 5—Weight percent Mo as a function of distance (m) across a dendrite (from center to edge) for the following time sequences at 1100 °C: 0 and 10 ks; and 1100 °C/10 ks + 1200 °C/30 and 70 ks.

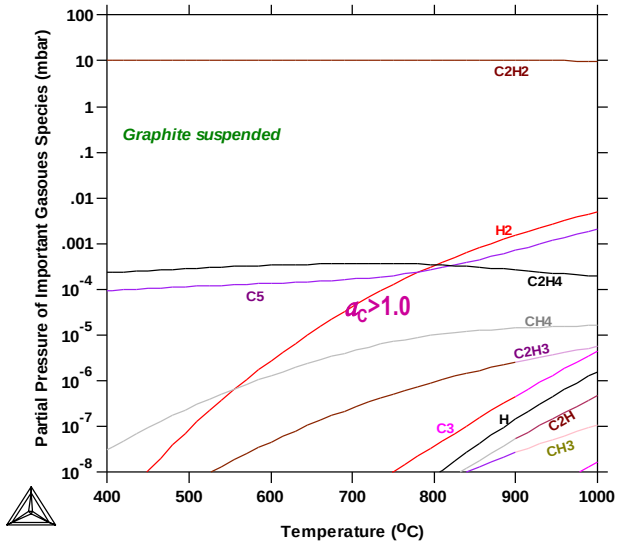
First heat treatment simulated at 1100°C (below incipient melting temp).
But incipient melting temp changes with chemical profile. In second case calculated a new incipient melting temp after 10,000 secs of 1275°C.
Significant improvement of the alloy homogeneity was predicted even after only 8.33 hrs (30,000 secs) @1200°C after the initial 10,000 secs @ 1100°C.

Example: Heat Treatment

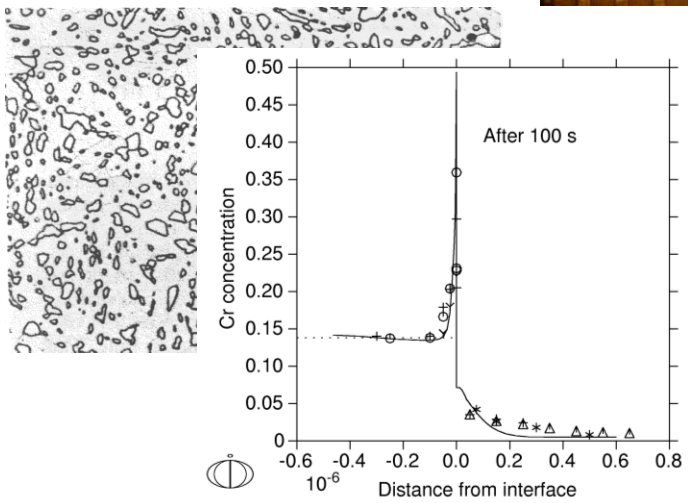
Applications to a wide range of heat treatment related simulations, e.g. to calculate:

- Gas phase reactions
- Equilibrium between alloy and gas phase as a function of temperature and composition
- Predict formation of phases / volume-fractions etc.
- Oxide scale formation

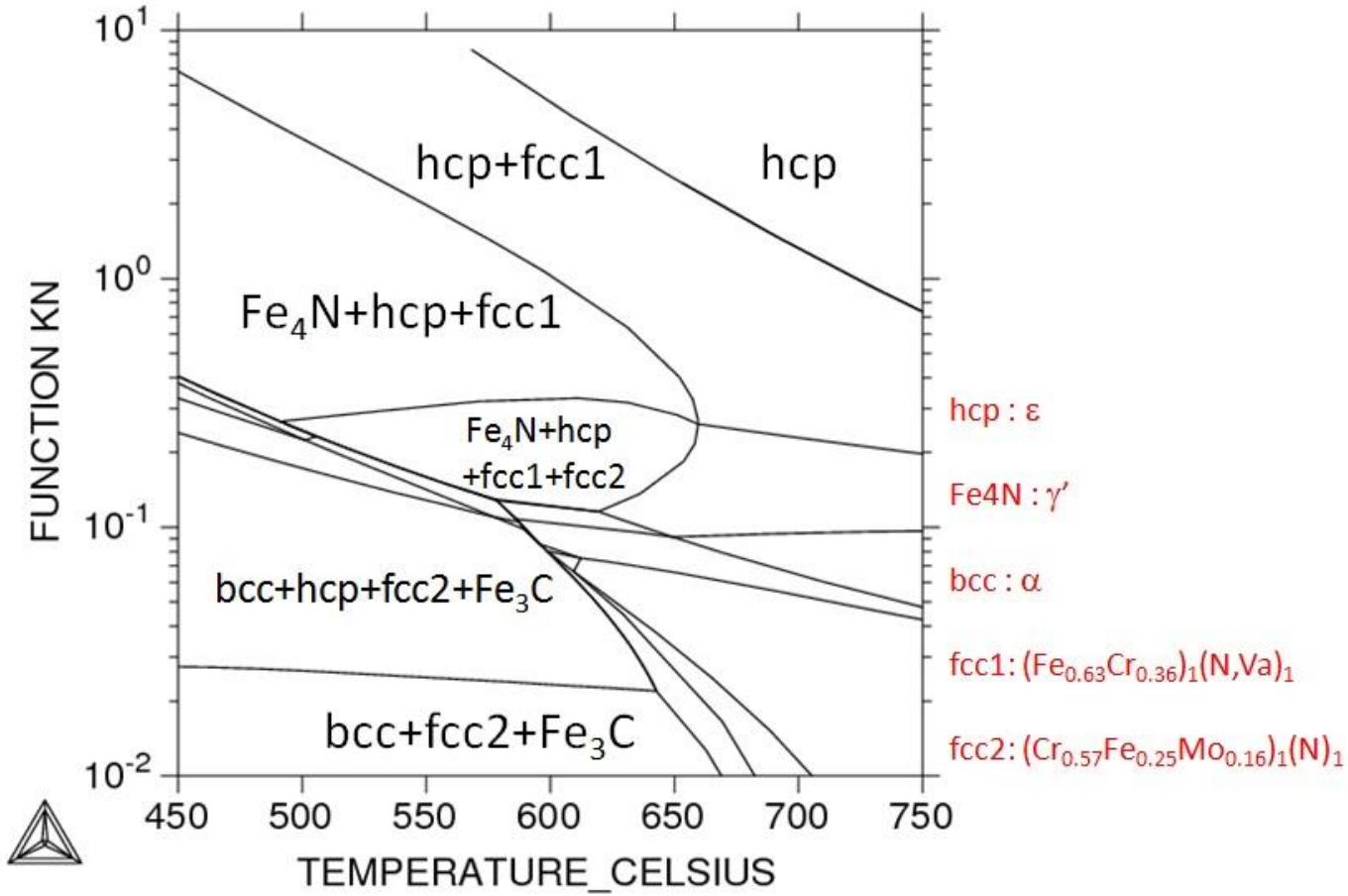
Decomposition of Acetylene at 10 mbar



Carbide dissolution



Example: Calculated Lehrer diagram



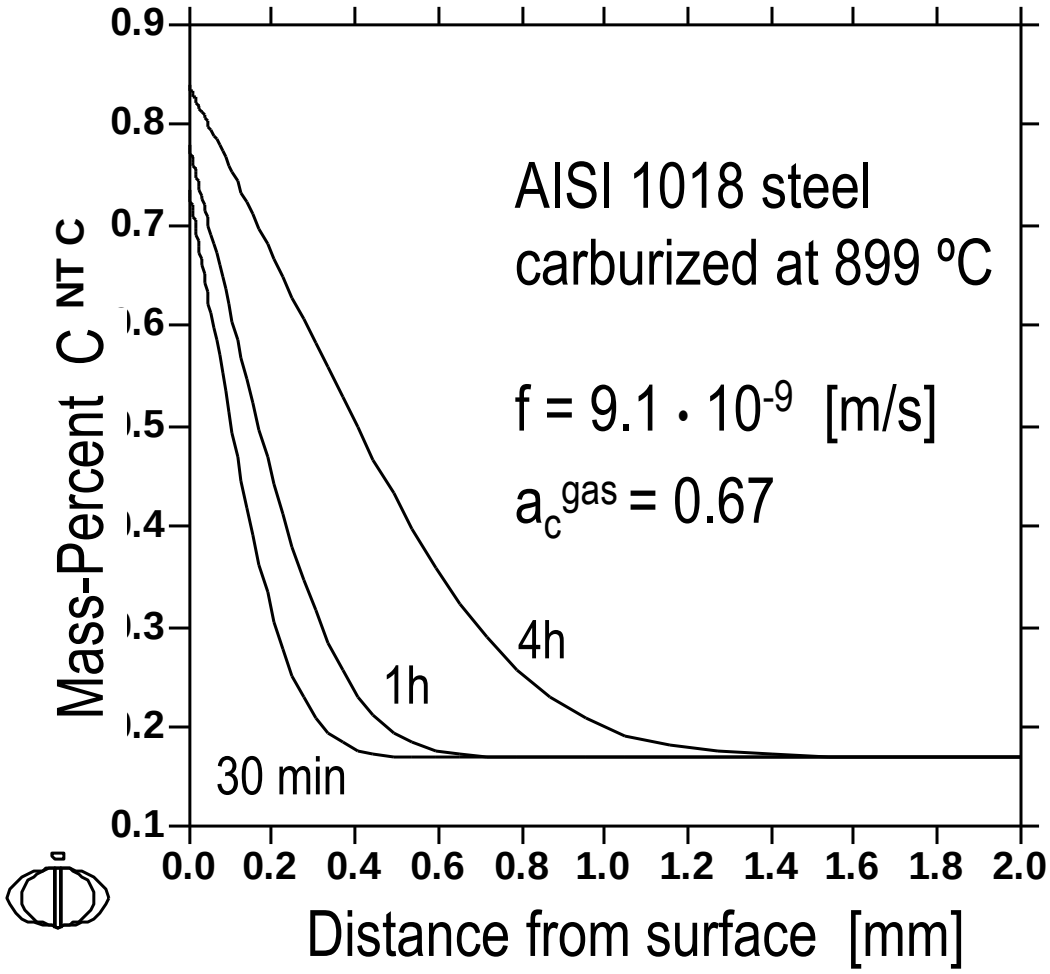
Example: Carburization of highly alloyed steels (1)

Use of activity-flux function in order to account for “surface reaction”.

$$J_c = f\,(a_c^{gas} - a_c^{surf})$$

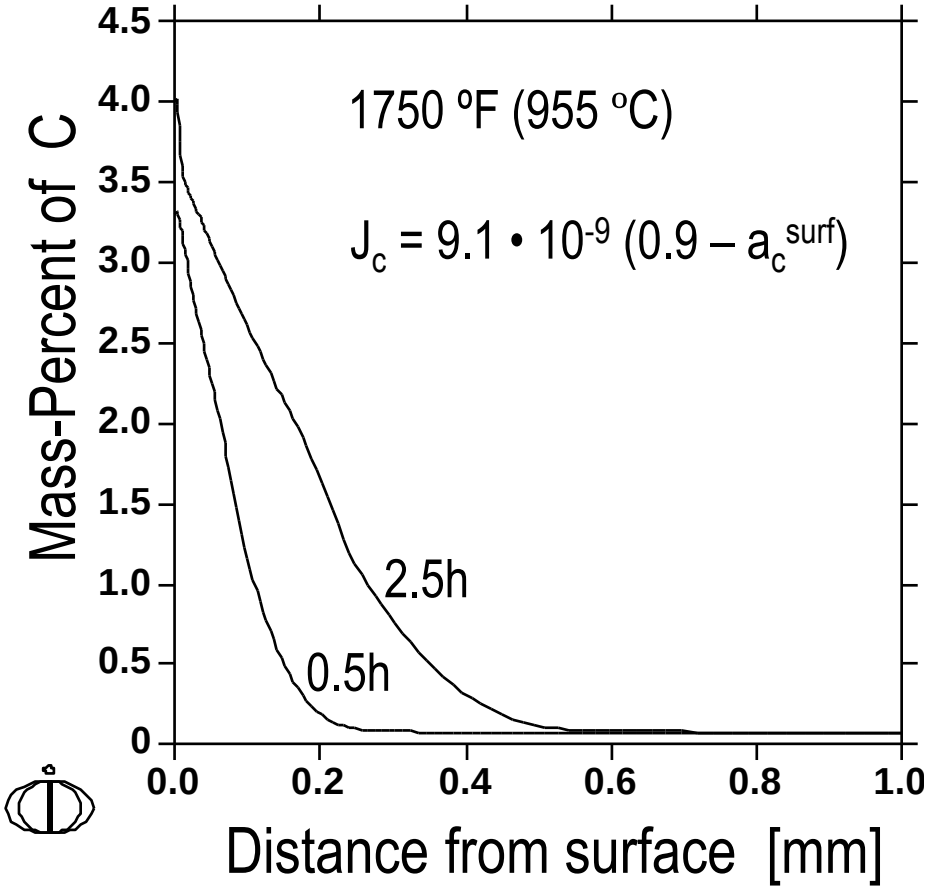
where f is a mass-transfer coefficient that needs to be determined for each case.

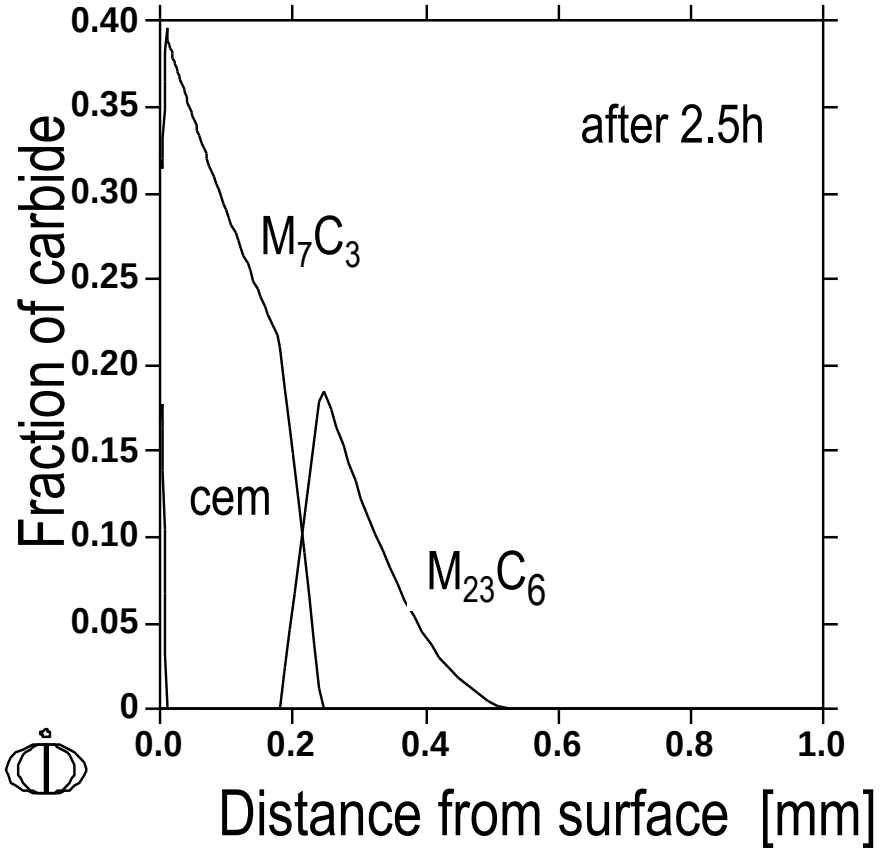
The “surface-reaction” taking place at the steel surface (and the mass-transfer coefficient) is believed to be strongly affected by pressure.



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

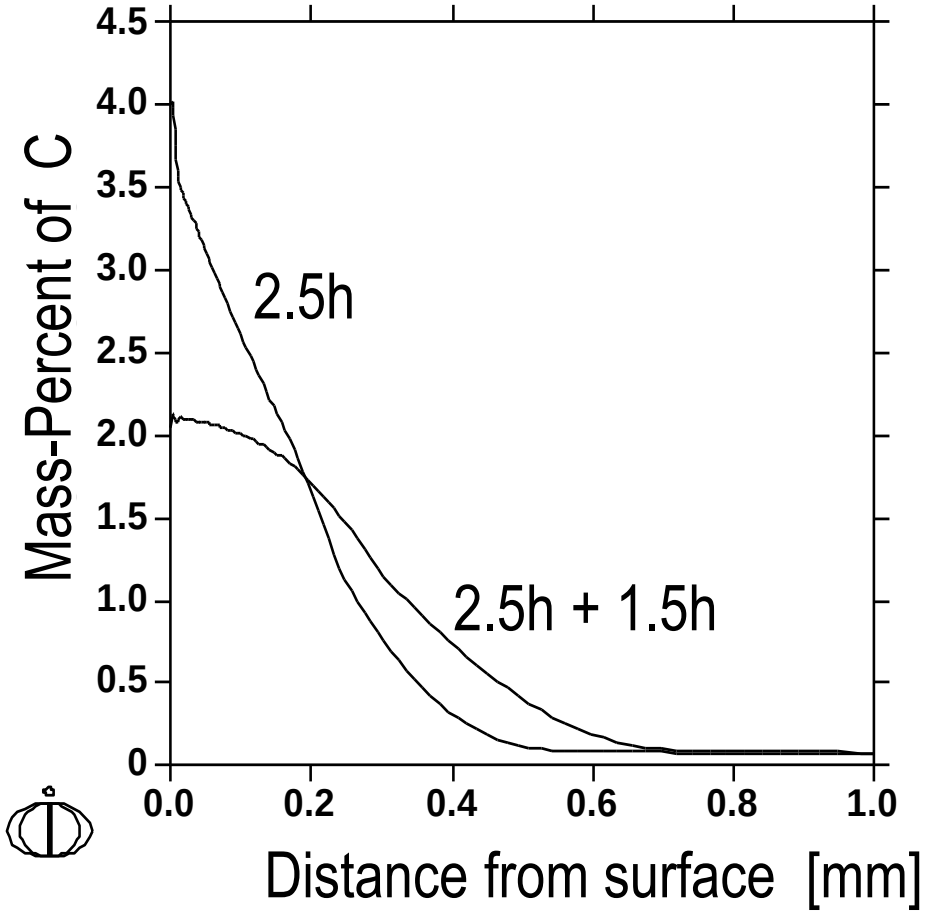
An example involving a complex alloy where alloying elements will tend to form carbides at high C-activities.





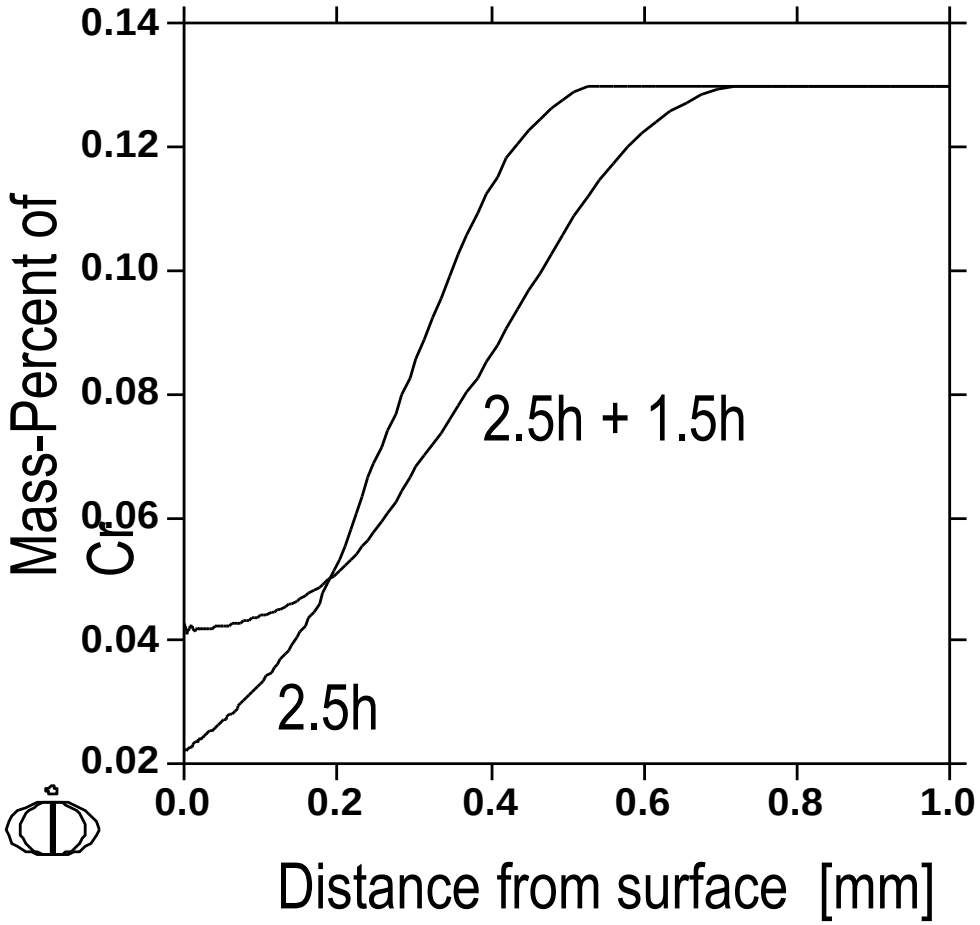
Example: Fe-13Cr-5Co-3Ni-2Mo-0.07C (2)

Adding a 1.5h “diffusion step”.



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

Cr depletion in the FCC matrix.



Example: Fe-13Cr-5Co-3Ni-2Mo-0.07C (4)

Validation is important!

Complements experiments, does not replace the need to do them.

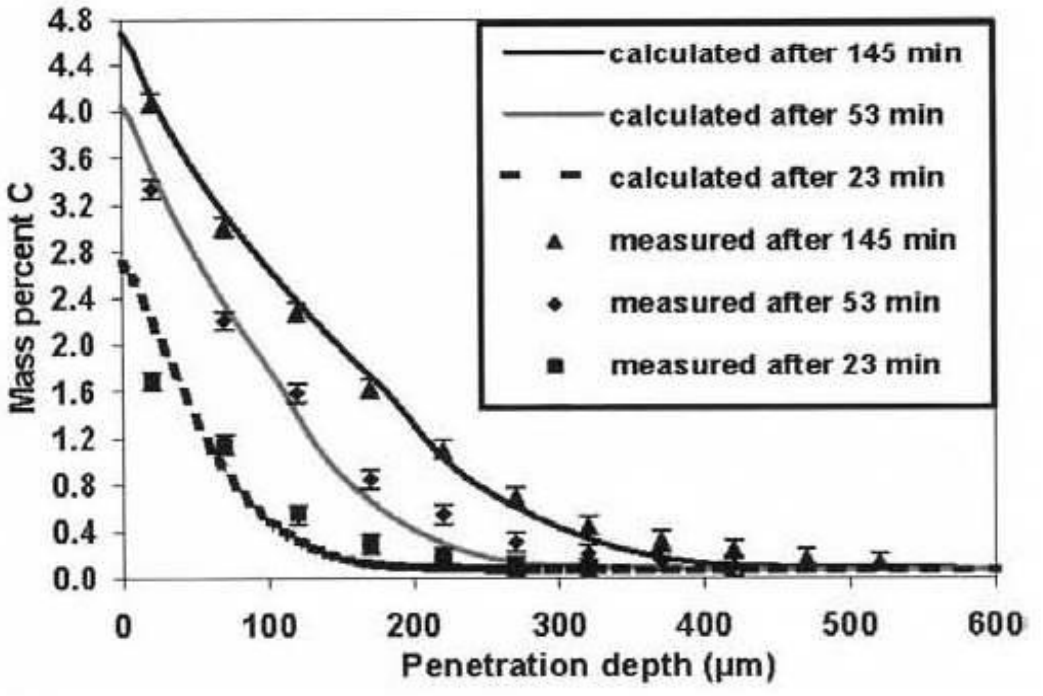
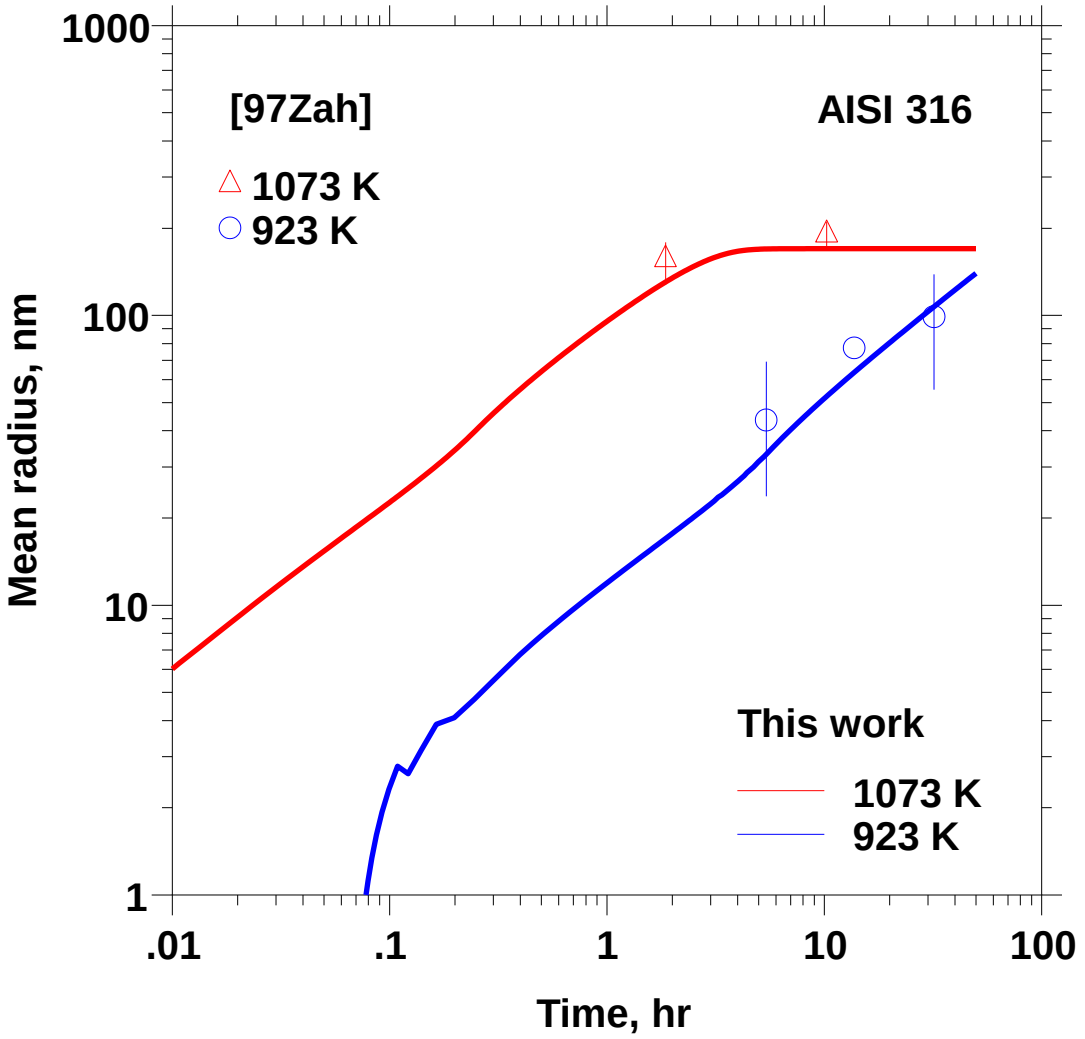


Fig. 16—Evolution of the experimental and calculated carbon profiles of three samples, of the Fe-13Cr-5Co-3Ni-2Mo-0.07C grade, carburized in the same conditions during 23, 53 and 145 min at 955 °C.

Turpin et al., Met. Trans. A ***36*** *(2005), pp. 2751-60*

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

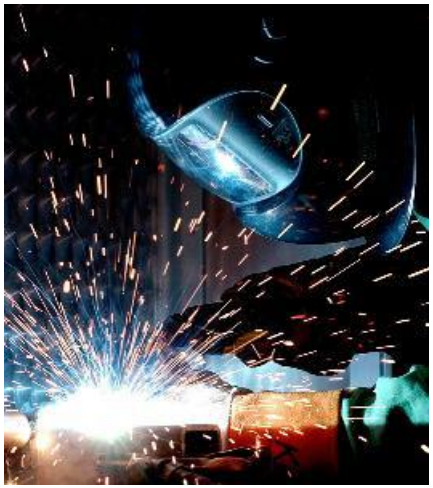
- γ-grainsize =100 μm
- σ = 0.3 J/m^2

@ 800 °C

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

Example: Welding and joining

CALPHAD based tools such as Thermo-Calc and DICTRA with suitable databases can predict:

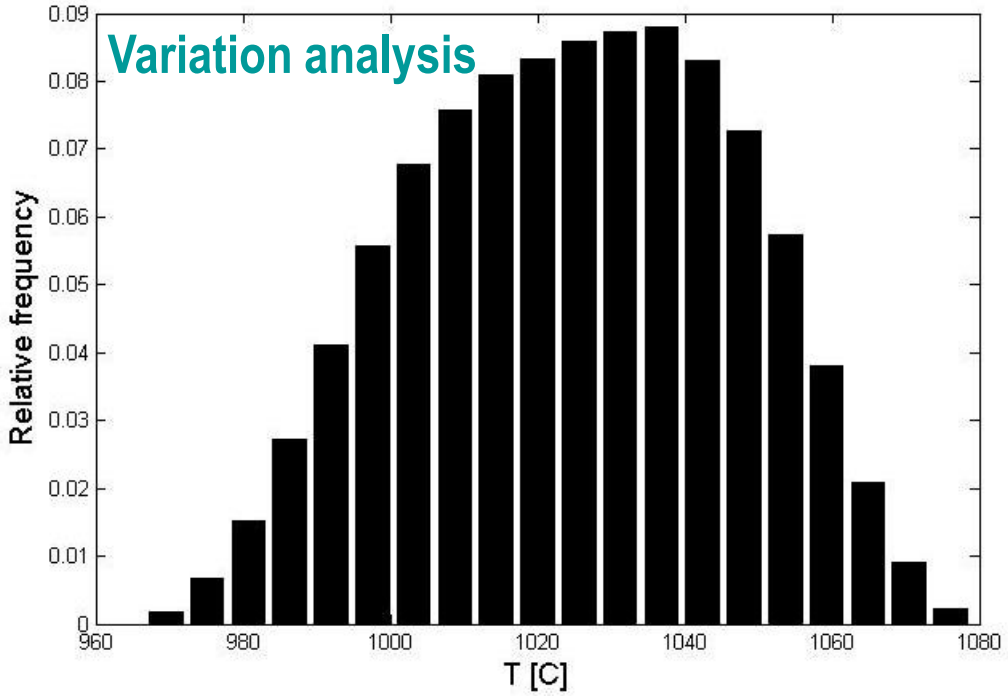


- ✓ Liquid-gas equilibrium
- ✓ Liquid-slag interactions
- ✓ Formation of inclusions
- ✓ Liquid-solid interactions
- ✓ Weld metal solidification paths and temperature ranges
- ✓ Microsegregation during solidification
- ✓ Prediction of HAZ grain boundary liquation
- ✓ Formation of precipitate phases at dissimilar welds
- ✓ Post weld heat treatment and more….

S. Babu, International Materials Reviews, 2009 Vol. 54 No. 6

Example: Composition control

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:

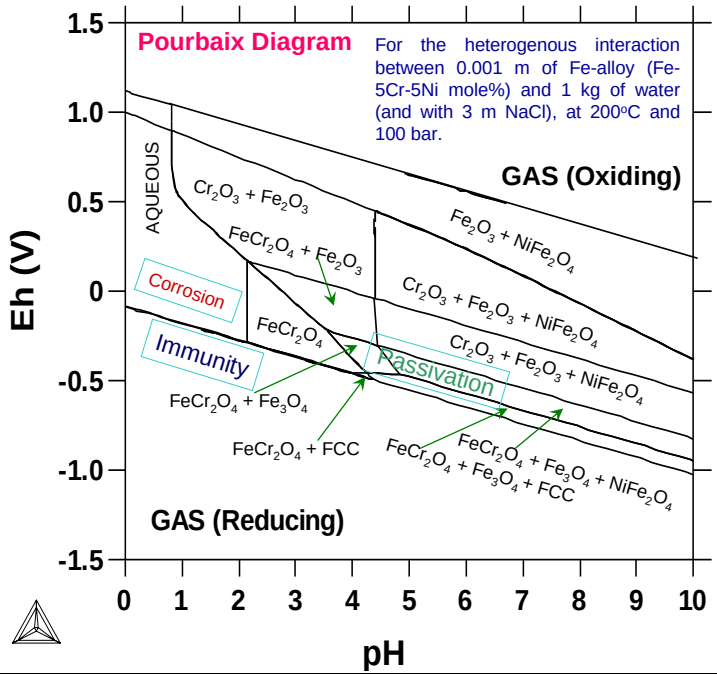
Fe	Base
Cr	23 – 27%
Ni	6 – 8%
Mo	3 – 5%
N	0.25 – 0.29%
C	0 – 0.03%

12^5 = 248832 calculations

Example: Corrosion

•These tools have also been applied to model different type of corrosion in alloys, e.g.

- ❑ High-temperature oxidation
- ❑ Salt corrosion
- ❑ Aqueous corrosion



Pourbaix diagram for the heterogeneous interaction between 0.001 m of steel [Fe-5Cr-5Ni mole%] and 1 kg of water (and with 3 m NaCl), at 200oC and 100 bar.

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?