Thermo-Calc Software

A master of science, engineering and entrepreneurship

Anders Engström

The Ågren Symposium 2017

Outline

1. Introduction
2. Science
3. Engineering
4. Entrepreneurship

Introduction – My interaction with John

Undergraduate	*1989 – 1991*	Lecturer
Ph.D. student	*1991 – 1996*	Supervisor
TCS employee	*2001 - present*	Chairman

Outline

1. Introduction
2. **Science**
3. Engineering
4. Entrepreneurship

A foundation

COMPUTER SIMULATIONS OF DIFFUSIONAL REACTIONS IN MULTICOMPONENT ALLOYS WITH SPECIAL APPLICATIONS TO STEEL

by

John Ågren

Doctoral thesis (1981)

1. A general treatment relating practical diffusion coefficients to so-called atomic mobilities and thermodynamic properties of a phase.
2. Numerical treatment of multicomponent diffusion in one-phase regions, i.e. solving a system of coupled PDEs.
3. Numerical treatment of diffusional reactions, i.e. solving a moving boundary type problem.
4. A vision directing future development.

Thermo-Calc Software

NUMERICAL TREATMENT OF DIFFUSIONAL REACTIONS IN MULTICOMPONENT ALLOYS

JOHN ÅGREN

Division of Physical Metallurgy, Royal Inst. of Technology, S-100 44 Stockholm, Sweden

(*Received* 6 *August* 1981; *accepted in revised form* 30 *September* 1981)

J. Phys. Chem. Solids vol. 43, no.4, (1982) pp. 385-391.

APPENDIX D

Construction of the computer program

(*a*) *General considerations.* The program will be based on the method that has been presented. As we do not want to impose still more restrictions on the model, the program must be constructed as flexible as possible. There should be no formal restrictions on the number of components on sublattices or on the number of phases involved. Of course, the actual computer capacity may put restrictions on how complex systems we can treat, but such restrictions should be easy to change in the program. Machine dependent facilities should be kept at a minimum and must be easy to change when the program is implemented on a different computer.

The user must be able to define any kind of initial conditions for the calculations. Boundary conditions should be possible to introduce in a most flexible way. Diffusion coefficients will be allowed to vary with temperature, composition, distance and time in an arbitrary way.

We also want to process the result of a simulation in different ways. For example, it should be possible for the user to get listings and graphical displays or hard copies of the results he is particularly interested in.

Sundman[12] has developed the Gibbs-Energy-System (GES), a FORTRAN subroutine package for the calculation of thermodynamic quantities with this philosophy in mind, and it seems natural to use his subroutines for all the thermodynamic manipulations needed in the program to be constructed. This package is based on a generalized regular solution type of model which was recently developed[13] and which is now adopted for the present purpose.

Furthermore, the program must be user friendly, i.e. it should be easy to handle for persons not used to computers. There should be a set of commands by which the user in a logical and simple way can define what he wants to have done.

(*b*) *Dynamic memory storage.* The requirements defined in the

(*d*) *Input and output.* The necessary input data for a simulation are:

(1) A thermodynamic description including molar volumes of the phases involved.

(2) Mobilities for the components in the different phases. The recently presented treatment of diffusion[1] yields expressions by which the diffusion coefficients can be calculated from the so-called mobilities and the thermodynamic properties of a phase. This is done automatically by the program.

(3) Geometrical exponent, m (is put to zero if no value is specified).

(4) Initial grid point coordinates in each phase.

(5) Initial compositions at the different grid points.

(6) Temperature as a function of time.

It is also possible to specify boundary conditions at the outer boundaries. If no conditions are specified, the fluxes of each component are put to zero at the outer boundaries. This condition means that the system is treated as a closed system.

The output is controlled by the user by different commands so that only data which are asked for are displayed. All the input data or parts thereof and their variation with time can be displayed.

A special feature is the possibility of saving on file a copy of the workspace. It is thus possible to terminate a simulation at any moment, save the actual status and continue the simulation from this moment at a later occasion by simply reading the file where the workspace was saved.

Diffusion Module (DICTRA)

Thermo-Calc Software

CALCULATE

Homogenization of alloys

Growth/dissolution of precipitate phases

Coarsening, or Ostwald ripening, of precipitate phases

Microsegregation during solidification

Interdiffusion in compounds, e.g. coating systems

Carburization, nitriding and carbonitriding of high-temperature alloys and steels

Influence of chemistry on diffusion coefficients in an alloy

Diffusion in a **temperature gradient**

Diffusion in **ordered** and **ionic/oxide phases**

EASY TO USE

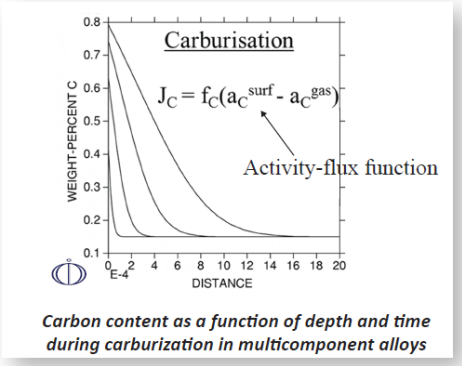
The Diffusion module makes modeling multicomponent diffusion controlled transformations simple and accessible, so you don't need to be an expert in computational thermodynamics and kinetics to use it. It uses command- based scripts, and examples of the most common kinds of problems are provided with the software.

PLATFORM

Windows, **Linux** and **Mac OS**

The Diffusion Module (DICTRA)

The Diffusion Module (DICTRA) is a unique add-on module within Thermo-Calc for the accurate simulation of diffusion controlled reactions in multicomponent alloy systems. The Diffusion module is based on the numerical solution of the multicomponent diffusion equations and the CALPHAD approach.



Carbon content as a function of depth and time during carburization in multicomponent alloys

Evolution

The Diffusion module was originally developed through a collaboration of the Royal Institute of Technology in Stockholm, Sweden, and the Max Plank Institute, Germany, and was first licensed commercially in 1992. Today, nearly 30% of Thermo-Calc customers add this module to their license in order to consider the influence of kinetics in their research.

Consistently Maintained and Updated

The Diffusion module has been consistently updated and improved since its release to satisfy the evolving needs of our user-base. It has now been integrated as a module within Thermo-Calc and, as such, is now on a two-times-per-year release cycle. Customers with a maintenance and support subscription for the Diffusion module receive these updates for free.

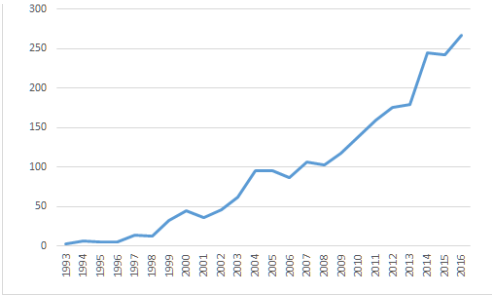
Technical Support and Training

The Diffusion module is backed by a dedicated customer technical support team. We also have agents around the world, as well as a subsidiary in the USA, who provide local customer support. Training courses are offered twice a year in Stockholm, Sweden, and Pittsburgh, PA, USA, as well as other locations around the world.

High Quality Mobility Databases

In order to perform a diffusion simulation, both a thermodynamic and

DICTRA Scientific publications



499 Sites

42 Countries

A foundation

COMPUTER SIMULATIONS OF DIFFUSIONAL REACTIONS IN MULTICOMPONENT ALLOYS WITH SPECIAL APPLICATIONS TO STEEL

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A foundation

Thermo-Calc Software

DIFFUSION IN PHASES WITH SEVERAL COMPONENTS AND SUBLATTICES

JOHN ÅGREN

Division of Physical Metallurgy, Royal Inst. of Technology, S-100 44 Stockholm, Sweden

(*Received 5 August* 1981; *accepted in revised form* 30 *September* 1981)

J. Phys. Chem. Solids, v 43 (5), (1982), pp. 421-30.

Models for numerical treatment of multicomponent diffusion in simple phases

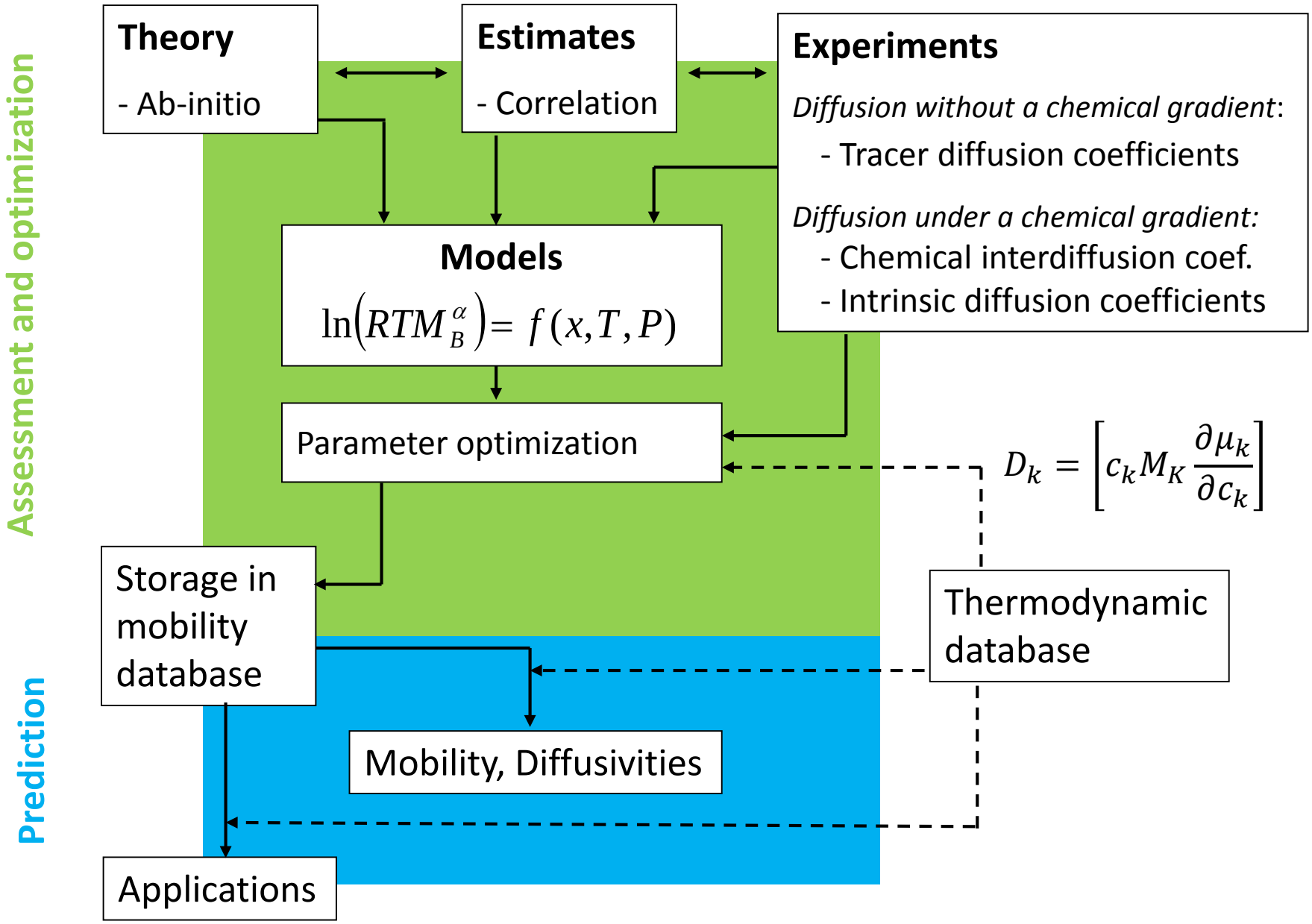
Jan-Olof Andersson and John Ågren
Division of Physical Metallurgy, Royal Institute of Technology, S-100 44 Stockholm, Sweden

(Received 30 August 1991; accepted for publication 27 April 1992)

A general formalism for multicomponent diffusion in simple phases is presented in some detail. The formalism is mainly based on previous work by various authors. The purpose of the present work is to develop the formalism to such an extent that it is suitable for implementation on a computer. Expressions for the multicomponent diffusion-coefficient matrix is given. The concentration dependence of the kinetic coefficients is discussed in terms of simple models.

J. Appl. Phys., 72 (4), (1992) pp. 1350-55.

Atomic Mobility Databases (*in a CALPHAD spirit*)



Atomic mobility databases (availability and use)

Today there are several databases available and used for different purposes.

13 Al 26.982 ALUMINIUM — ALUMINIUM »

26 Fe 55.845 IRON — IRON »

12 Mg 24.305 MAGNESIUM — MAGNESIUM »

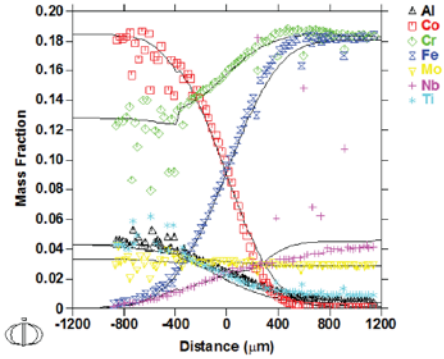
28 Ni 58.693 NICKEL — NICKEL »

22 Ti 47.867 TITANIUM — TITANIUM »

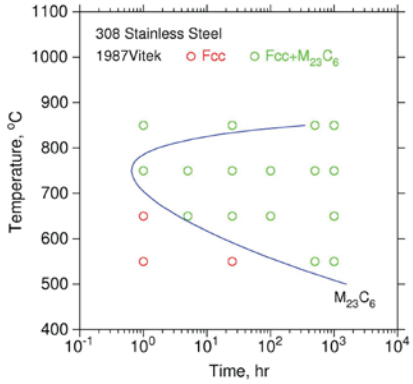
29 Cu 63.546 COPPER — COPPER »

SOLDERS »

OTHER MATERIALS »

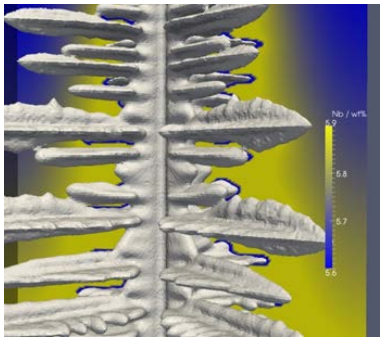


Diffusion simulations

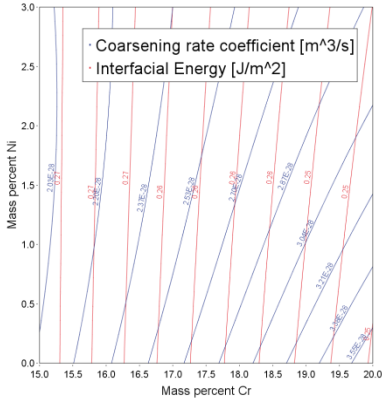


Precipitation simulations

Phase-Field



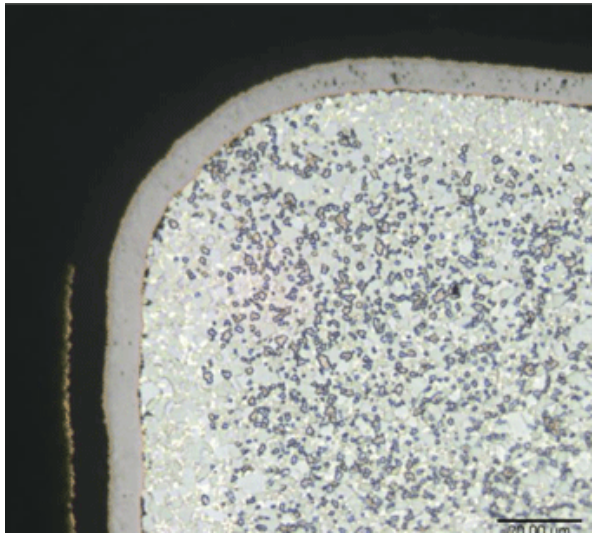
and more!



Diffusion in dispersed systems – My project!

Simulation of diffusion in multi-component dispersed systems, e.g.

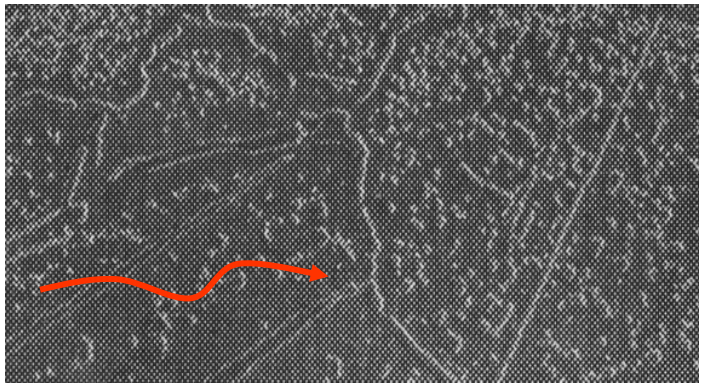
- ❑ Interdiffusion in compounds
- ❑ Gradient sintering
- ❑ Internal oxidation, etc.



Gradient sintered hard metal

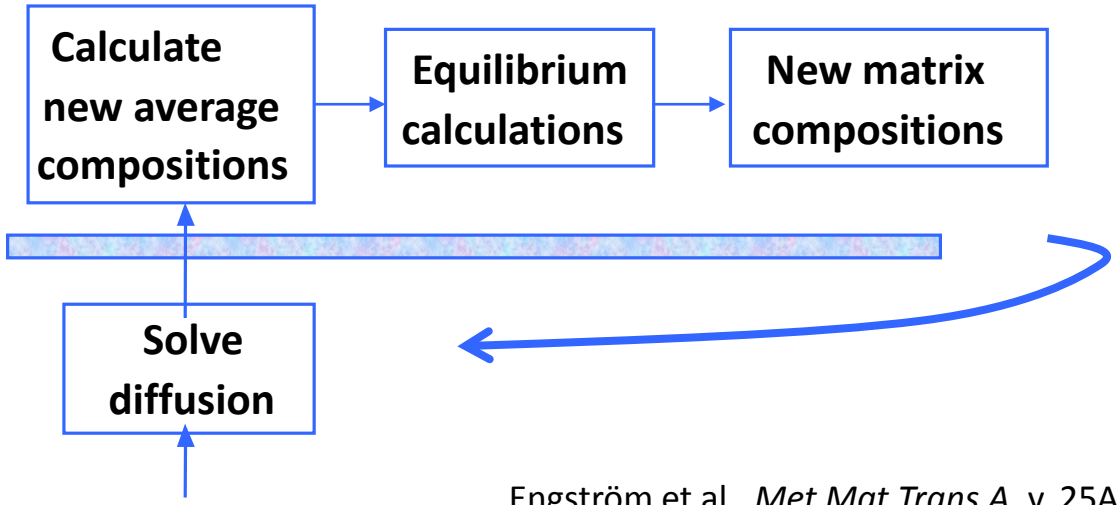
Diffusion in dispersed systems

Implemented model based on a method developed by Bongartz et al. (1980)



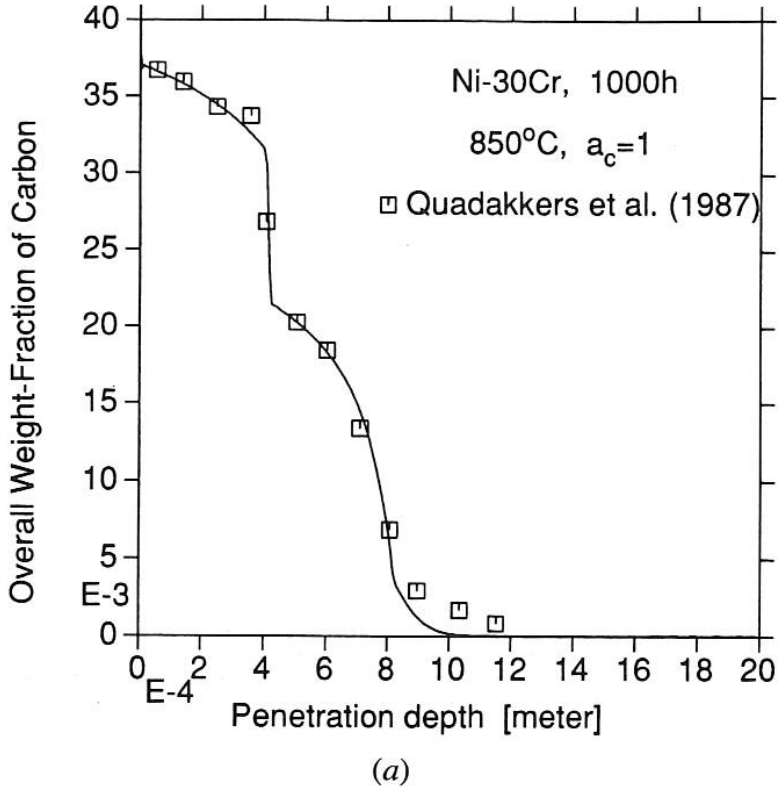
Assumptions:

- Diffusion takes place in the matrix phase only.
- Equilibrium holds locally in each node.

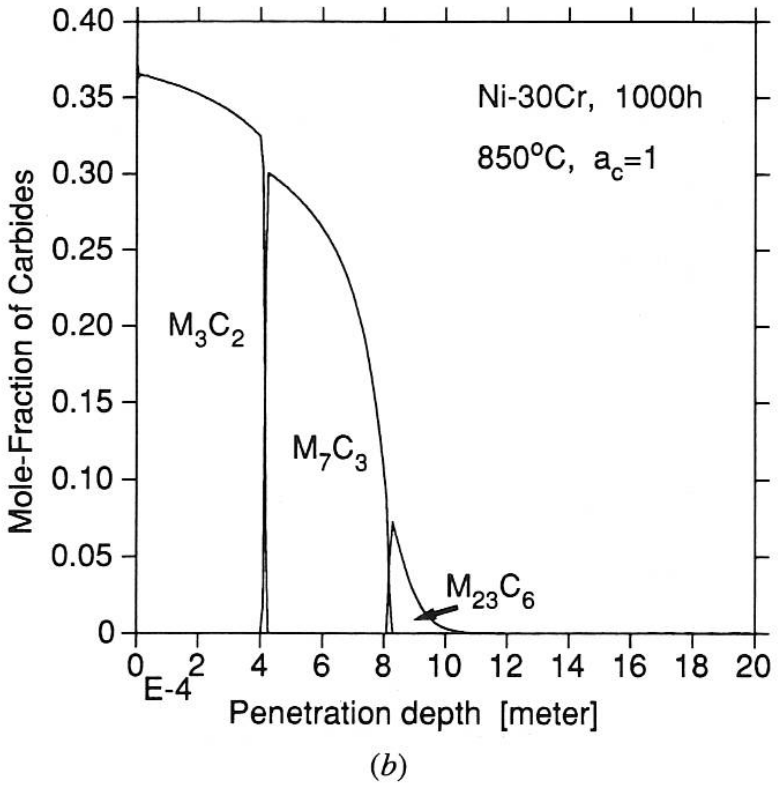


Engström et al., *Met Mat Trans A,* v. 25A (1994), p 1127.

Carburization of Ni-30%Cr alloy



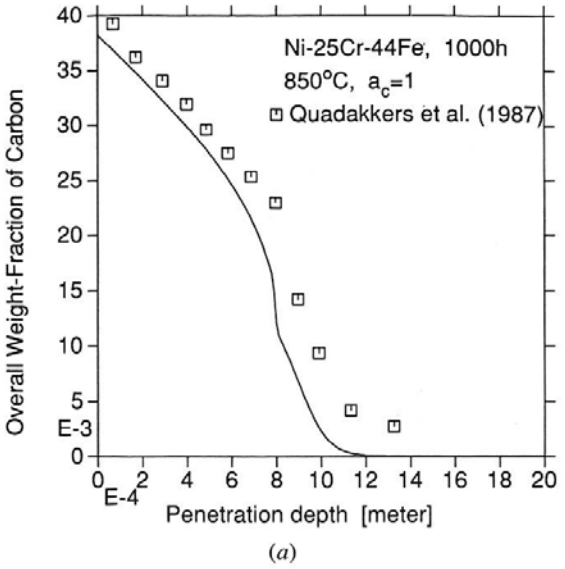
(a)

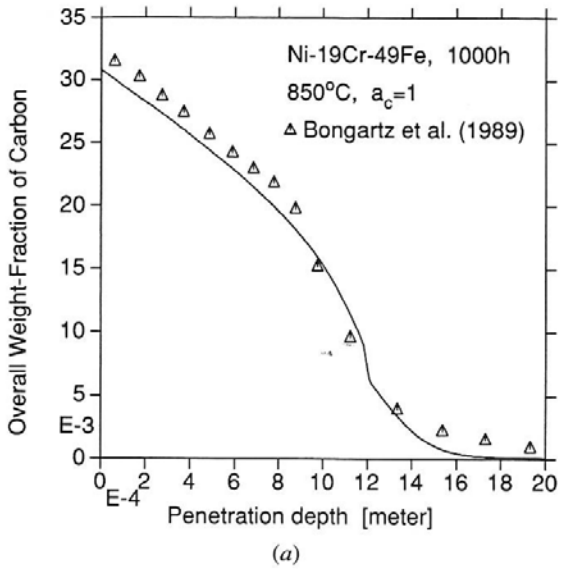


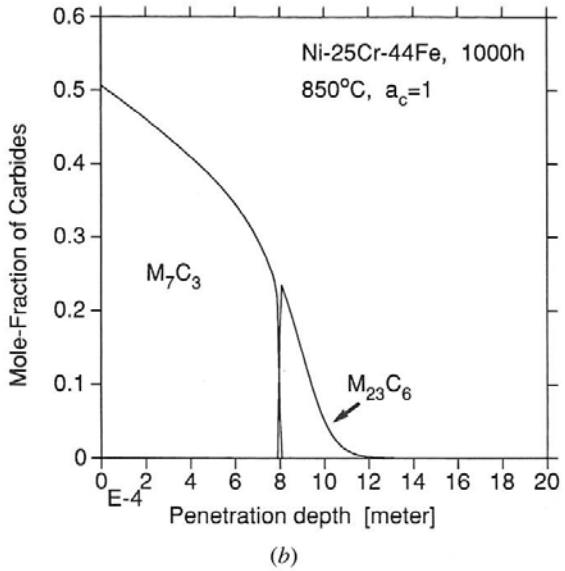
(b)

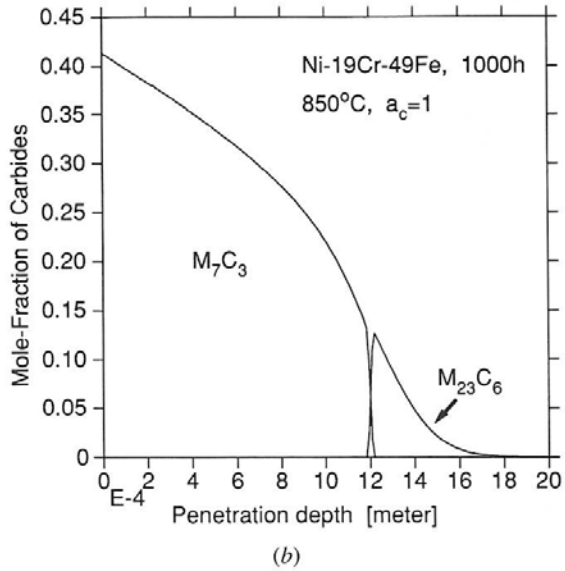
Engström et al., *Met Mat Trans A,* v. 25A (1994), p 1127.

Carburization of Ni-Cr-Fe alloys



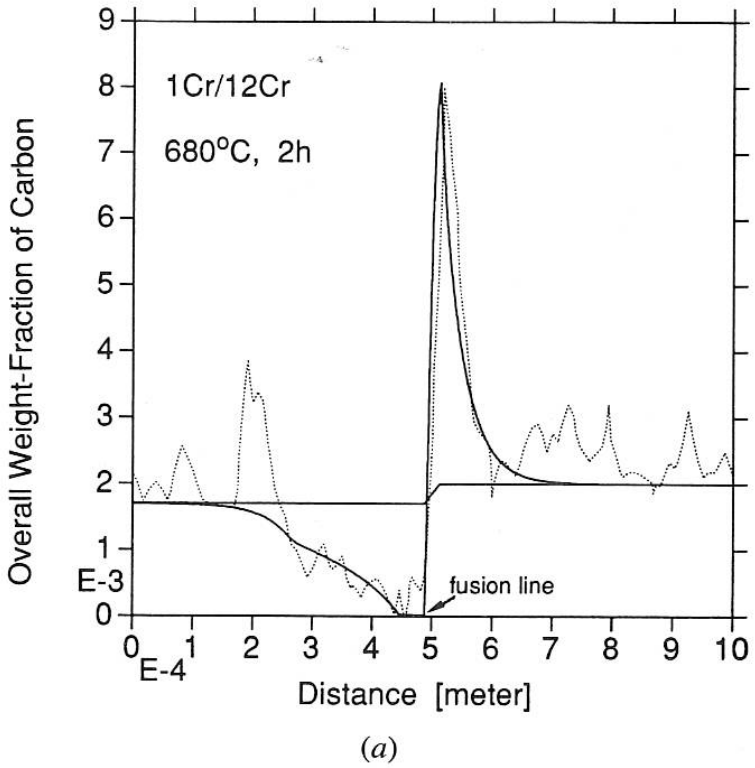




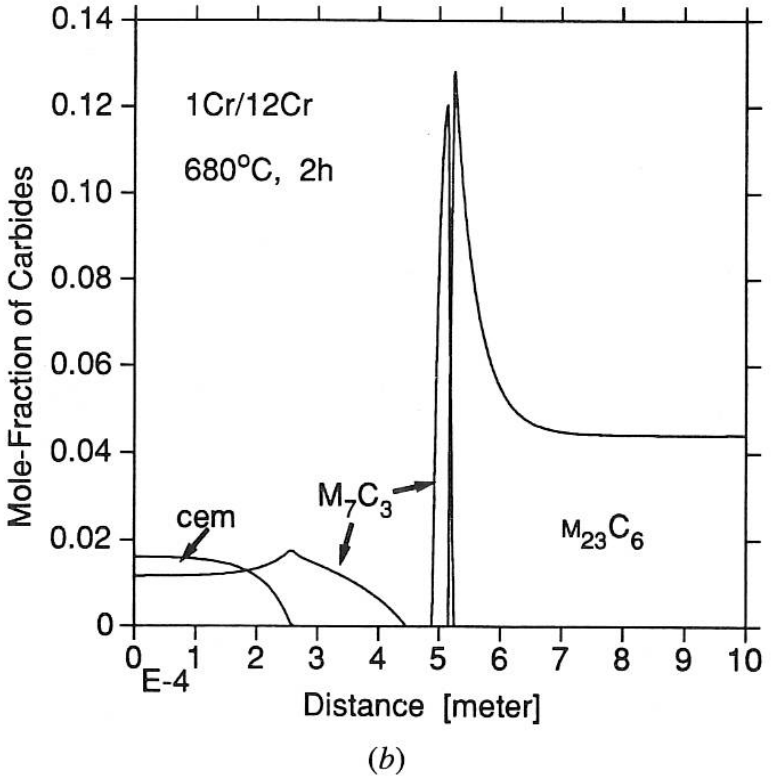


Engström et al., *Met Mat Trans A,* v. 25A (1994), p 1127.

Annealing of mismatched Chromium alloy weldment



(a)



(b)

Engström et al., *Met Mat Trans A,* v. 25A (1994), p 1127.

Ni-Cr-Al alloys

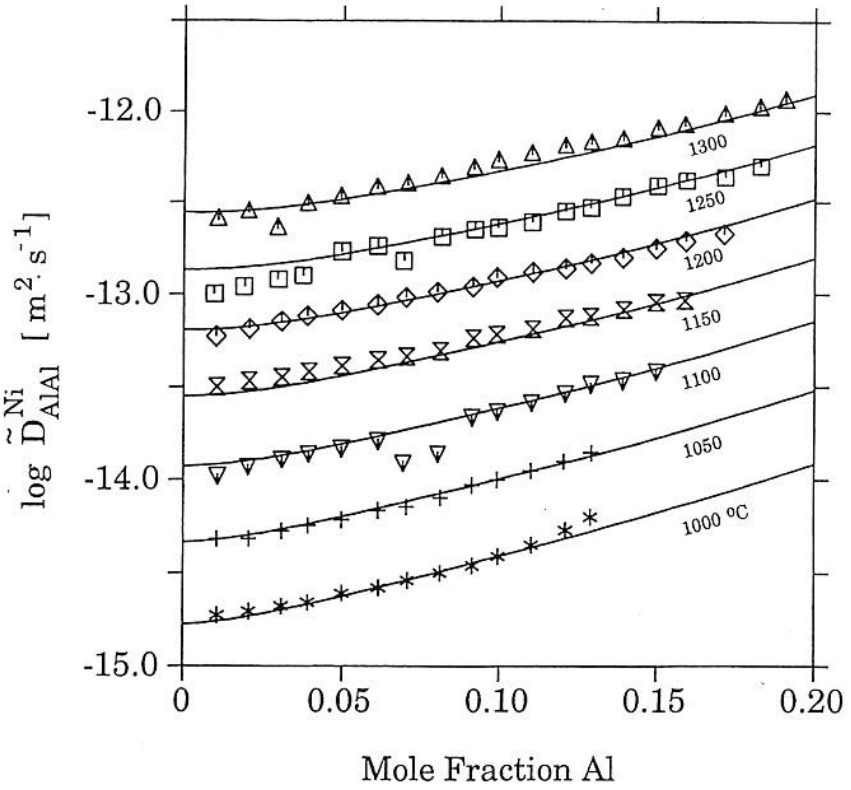


Fig. 1. The interdiffusion coefficient in the Ni –Al system as a function of the Al concentration at seven different temperatures. Comparison between calculated $\tilde{D}$ (lines) and experimental values [8].

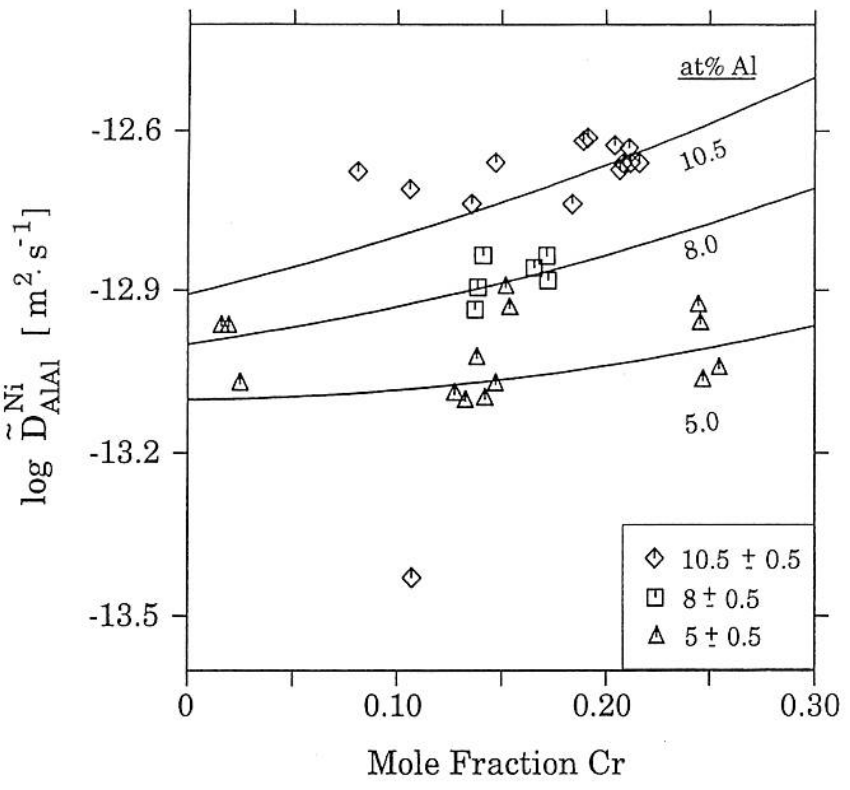
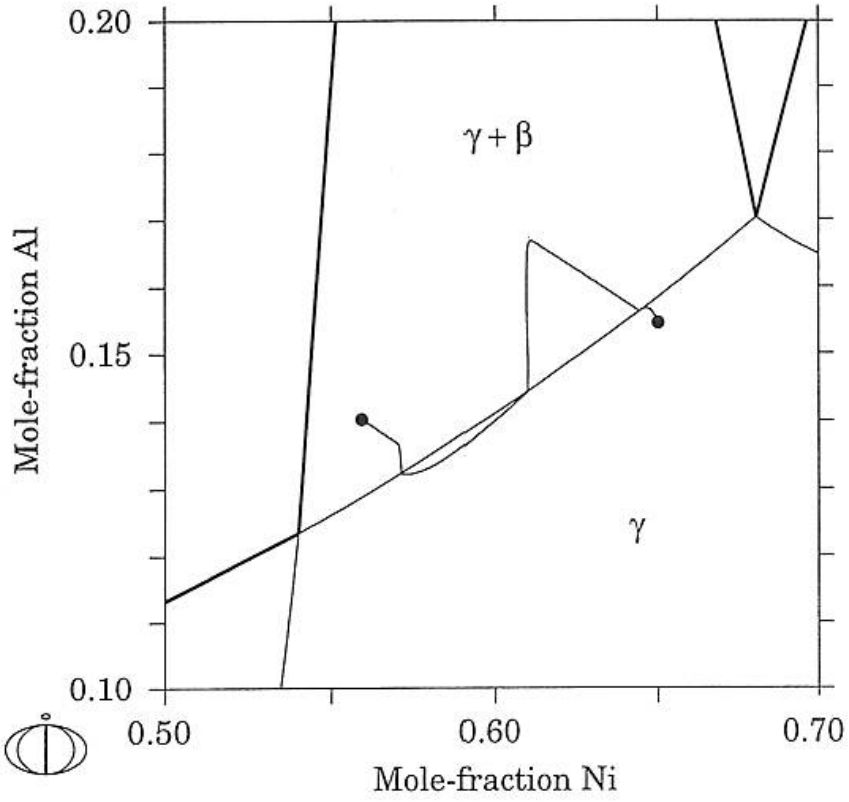
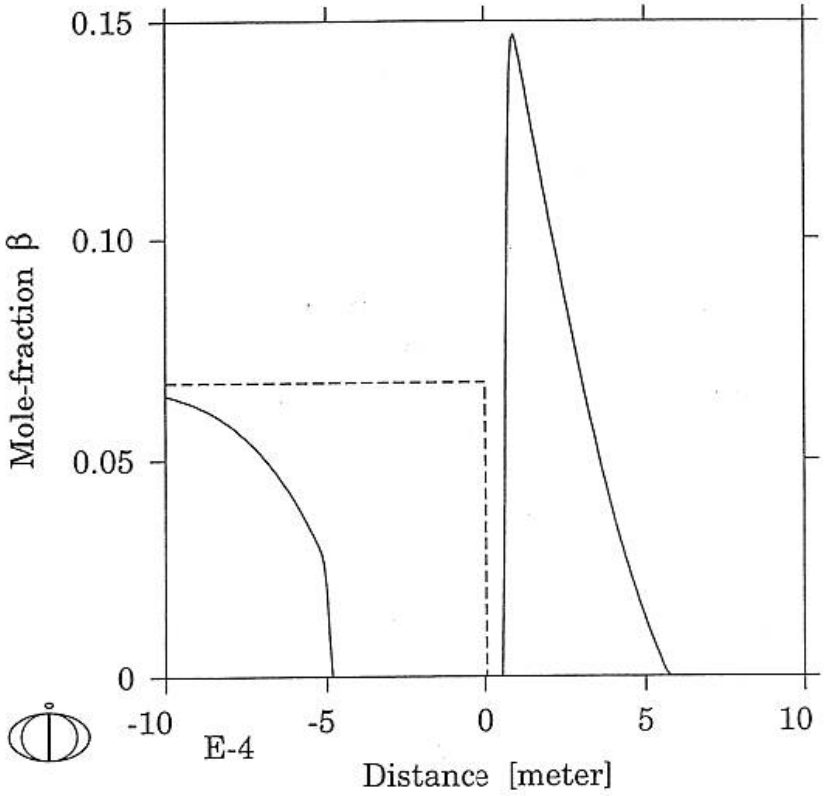


Fig. 2. The ternary interdiffusion coefficient $\tilde{D}^{Ni}_{AlAl}$ at 1200 °C as a function of the Cr concentration for three different Al concentrations. Comparison between calculated $\tilde{D}^{Ni}_{AlAl}$ (lines) and experimental values [9].

Engström and Ågren, *Z. Metallkd.,* v. 87 (1996), p. 92.

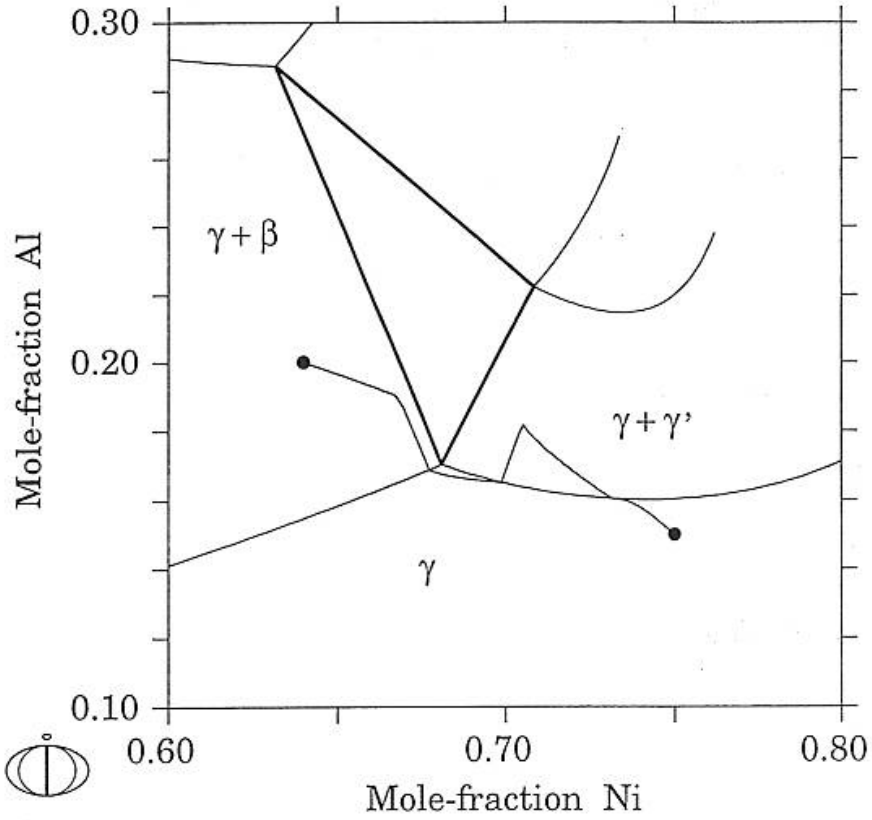
Ni-Cr-Al multiphase diffusion couples

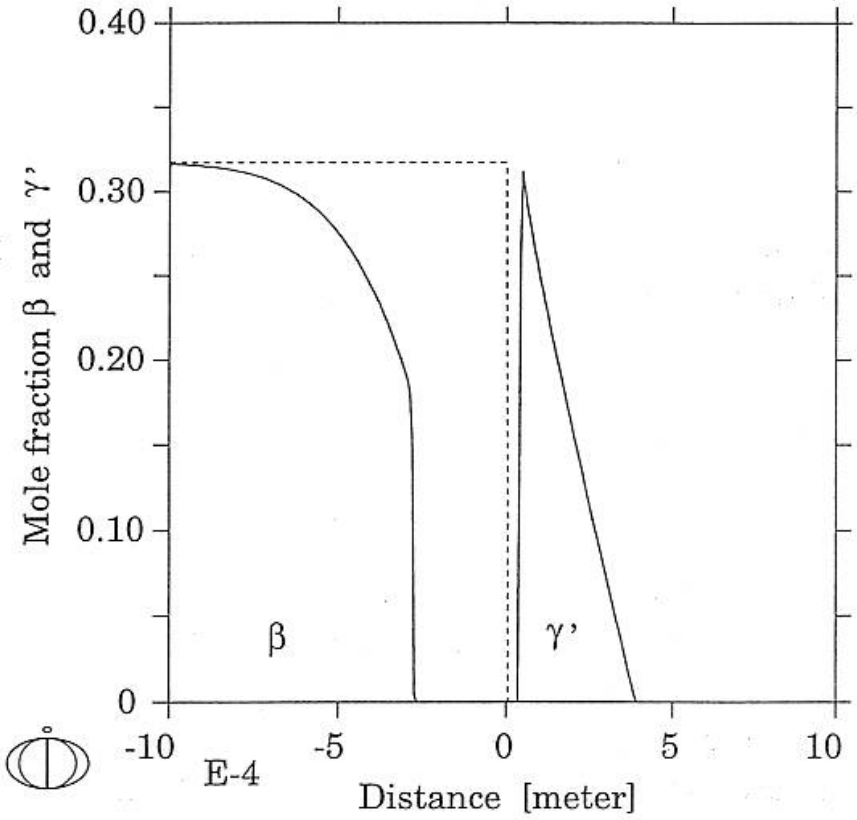




Engström et al., *Acta Mater.*, v. 45 (1997), p. 1189.

Ni-Cr-Al multiphase diffusion couples





Engström et al., *Acta Mater.*, v. 45 (1997), p. 1189.

Gradient sintering

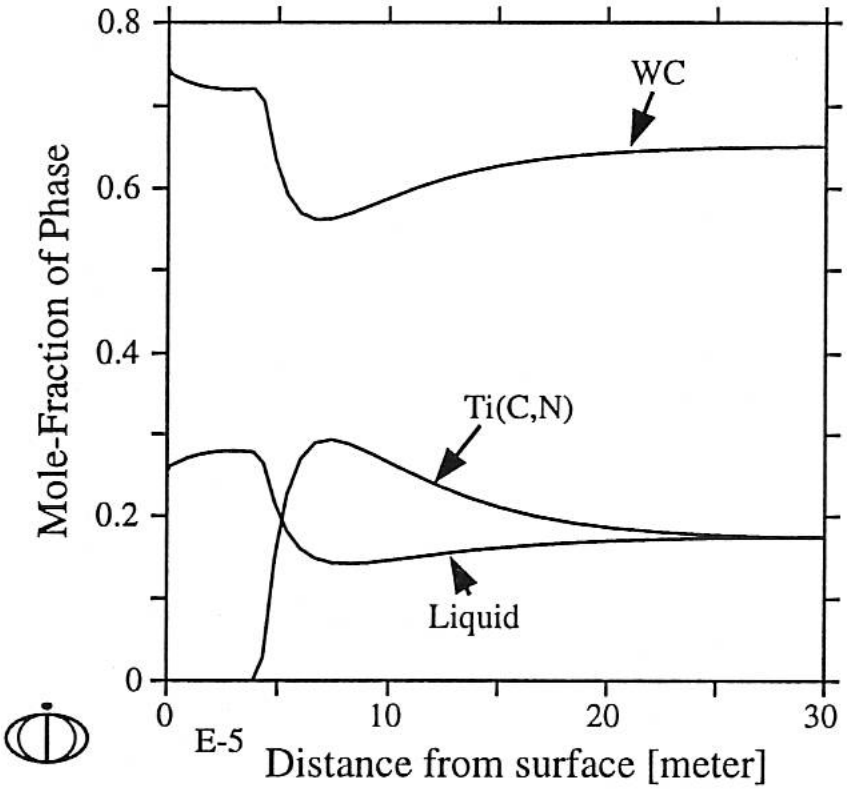


Fig. 4: Calculated mole fractions of the phases present in a typical cemented carbide alloy, W-9 wt pct Co-4.25 wt pct Ti-6.4 wt pct C-0.34 wt pct N after 1 h sintering in a nitrogen free atmosphere at 1540 ° C.

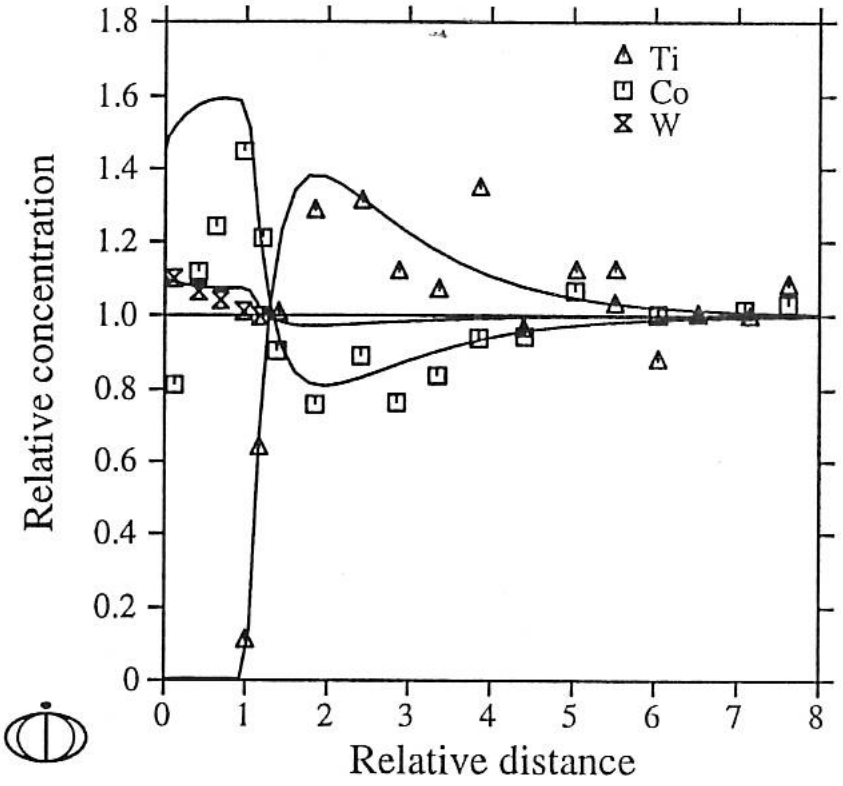


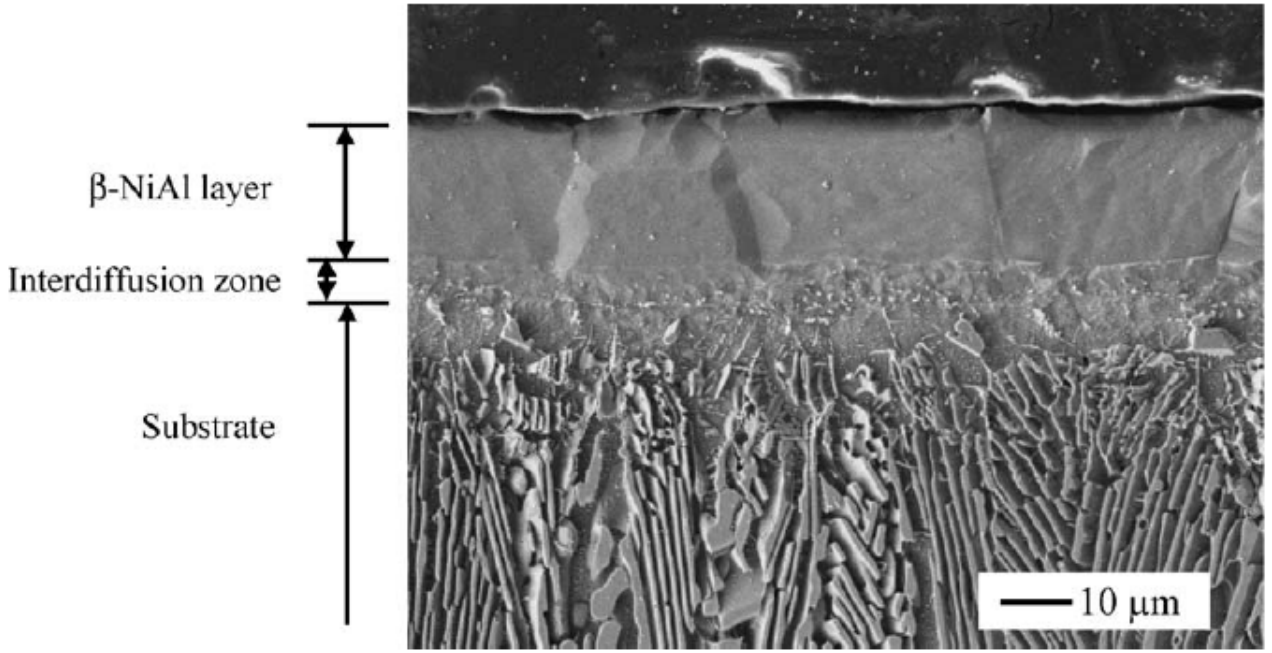
Fig. 5: Concentration profiles for Ti, Co and W after 1 h of sintering at 1540 °C in a nitrogen free atmosphere. The concentrations have been normalized against the initial concentration of each component whereas the distance has been normalized aginst the thicknes of the gradient zone. Symbols: experimental data from Ref. 18.

Engström and Ågren, *The Sefström Symposium* (1994)

More complex problems

Thermo-Calc Software

Coating degradation due to interdiffusion

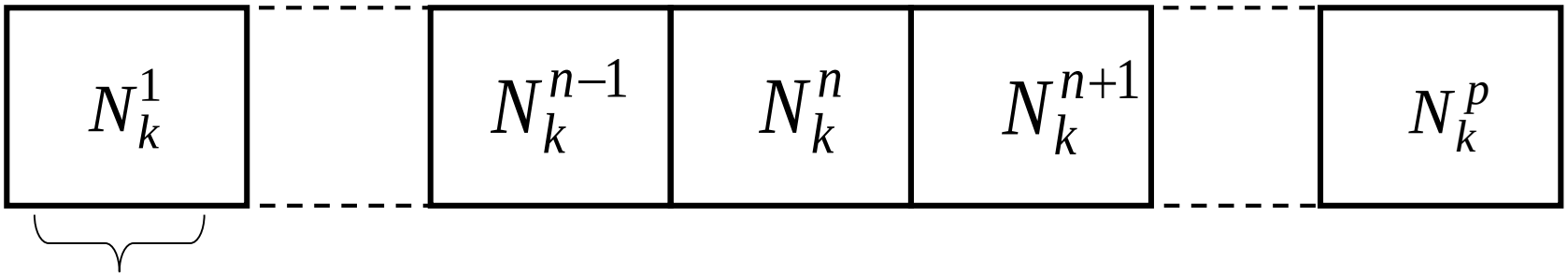


Yu et al., *Mater Sci. Eng*. A394 (2005) 43.

- Complex problem that involves solving a multicomponent diffusion problem in a multiphase region.
- Need for multicomponent kinetic data in β-NiAl, γ and γ'.

Homogenization model

Approach that allows us to account for diffusion in more than one phase.



Equilibrium calculation for each slice

Phase fractions
Phase compositions
Chemical potentials
Mobilities

Flux between slices "n-1" and "n"

$$J_k = \frac{-1}{V_m}\sqrt{\left[M_k x_k\right]_{n-1}^{eff}\left[M_k x_k\right]_n^{eff}}\,\frac{\Delta\mu_k}{\Delta z}$$

"Effective" $[M_k x_k]$ from combining rules

Larsson and Engström, *Acta. Mat., v.* 54 (2006), p. 2431.

Calculating effective [$M_k x_k$]

Thermo-Calc Software

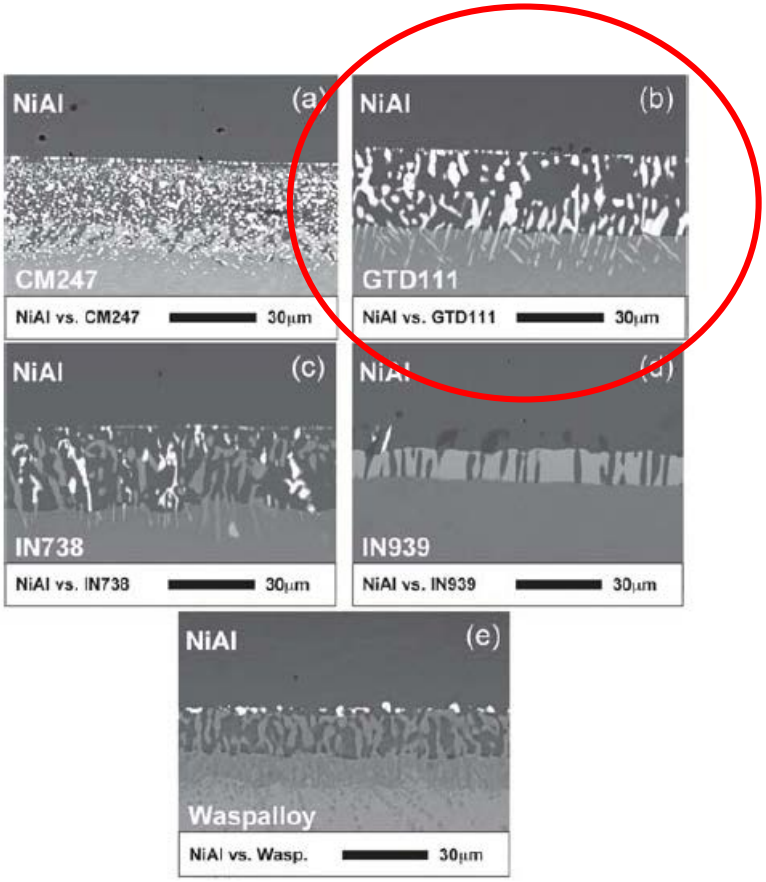
Combining rules are frequently used to determine an "effective" transport property in a multiphase mixture, from:

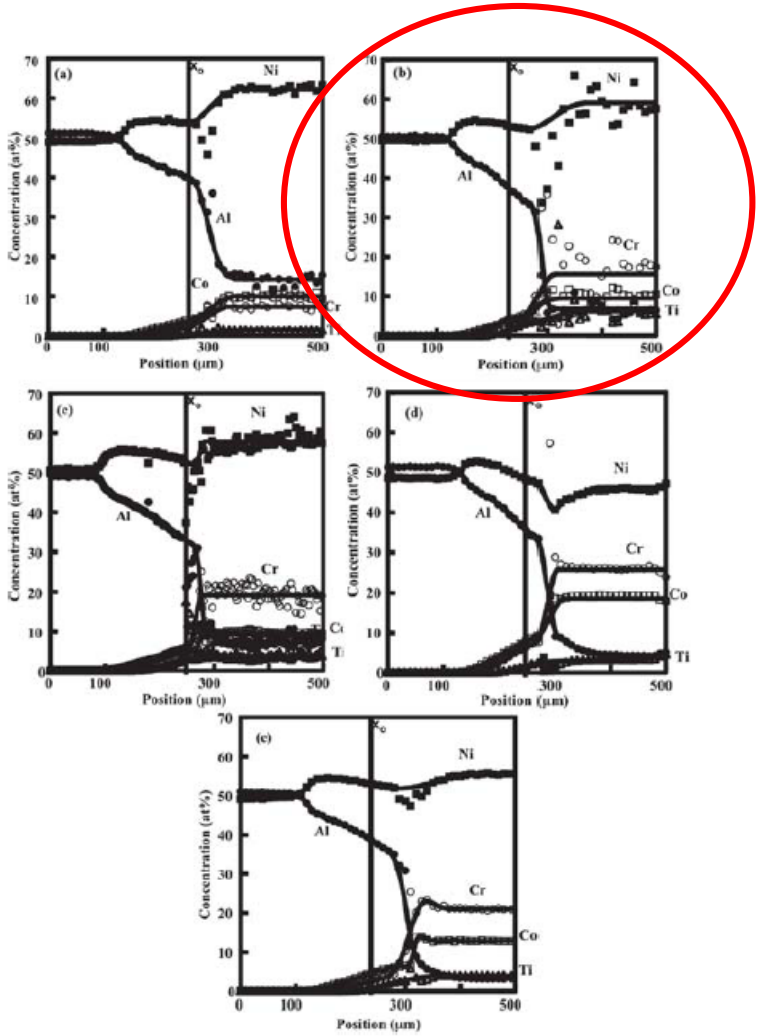
1) the transport properties in the individual phases,
2) the fraction of phases,
3) and sometimes also from the geometrical distribution.

Exact knowledge of the geometrical distribution is rarely known for a real case and it may be useful to study limiting cases or bounds (e.g. Wiener, Hashin-Shtrikman bounds).

Larsson and Engström, *Acta Mat.,* 54 (2006), p. 2431.

NiAl-coating / Ni-base superalloy system



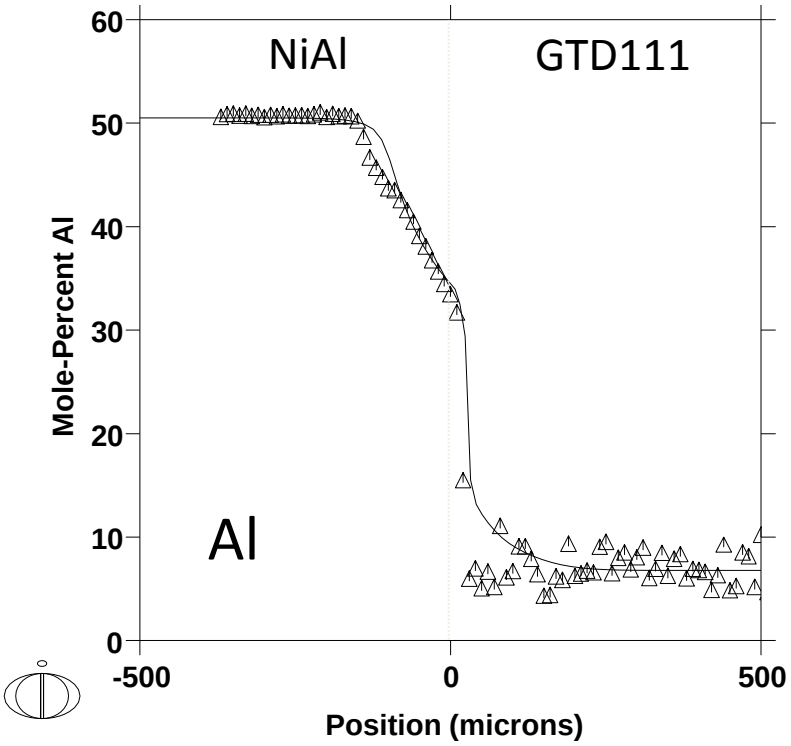


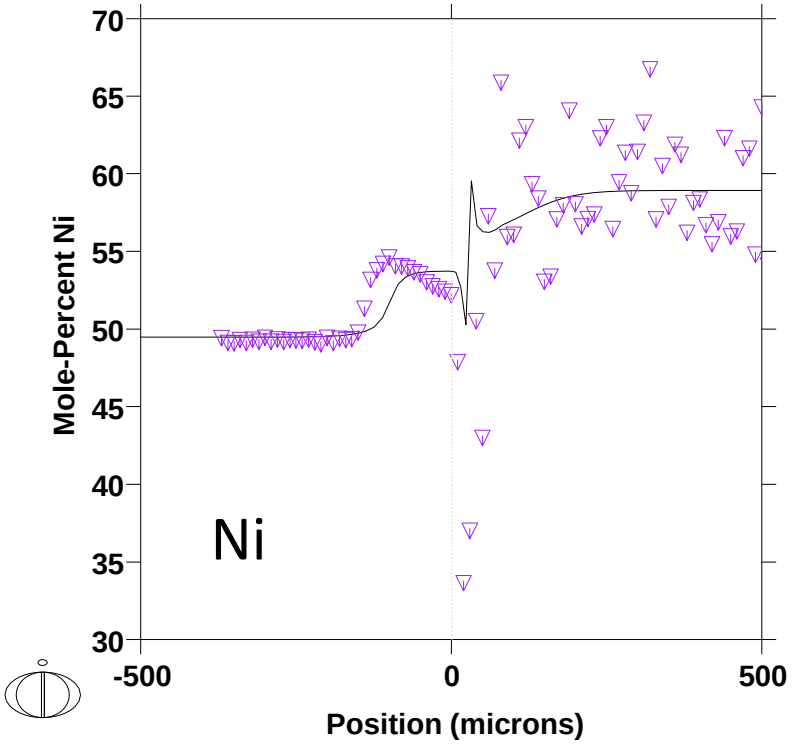
E. Perez, T. Patterson and Y. Sohn, *J. Phase Equilibria Diffus.,* v. 27(2006), pp. 659-64.

NiAl-coating / GTD111

	Ni	Al	C	Co	Cr	Mo	Ta	Ti	W
NiAl-Coating	Bal	50.5	-	-	-	-	-	-	-
GTD111	Bal	6.9	0.48	9.5	16.6	0.97	0.89	6.24	0.97

Temp. 1050°C
Time 96h





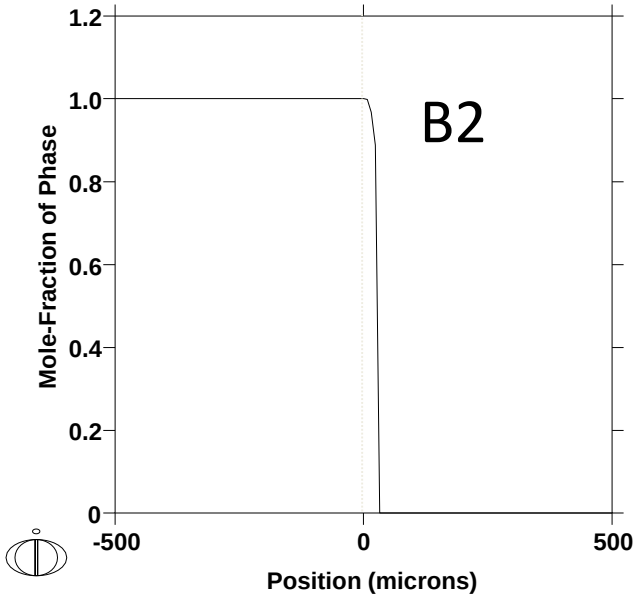
Rule of mixtures

$$\left[M_k x_k\right]^{eff} = \sum f^i \left[M_k x_k\right]^i$$

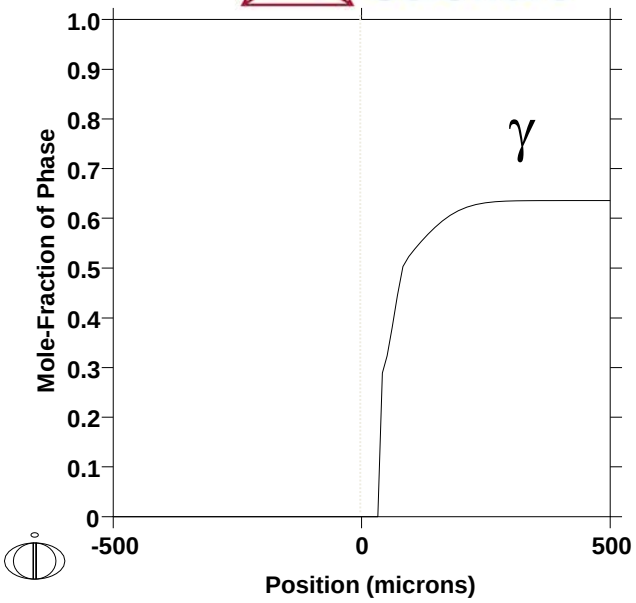
Symbols are experimental data from E. Perez, T. Patterson and Y. Sohn, J. Phase Equilibria Diffus., v 27 (2006), pp. 659-664.

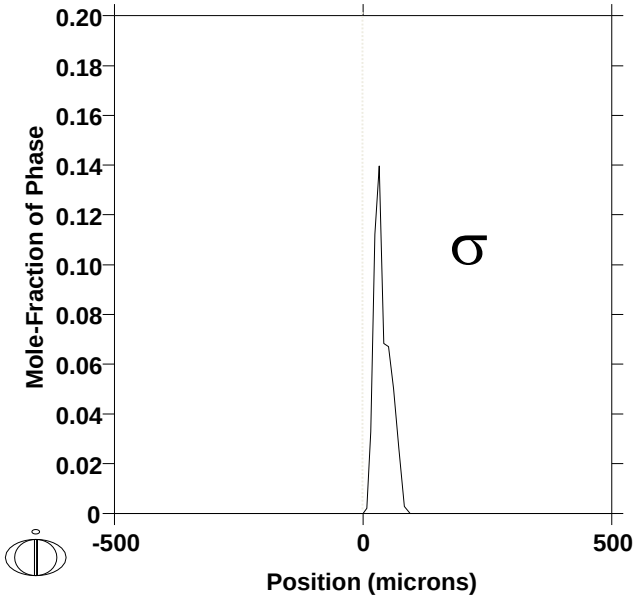
Engström et al., Advanced Materials Research Vol. 278 (2011) pp 198-203.

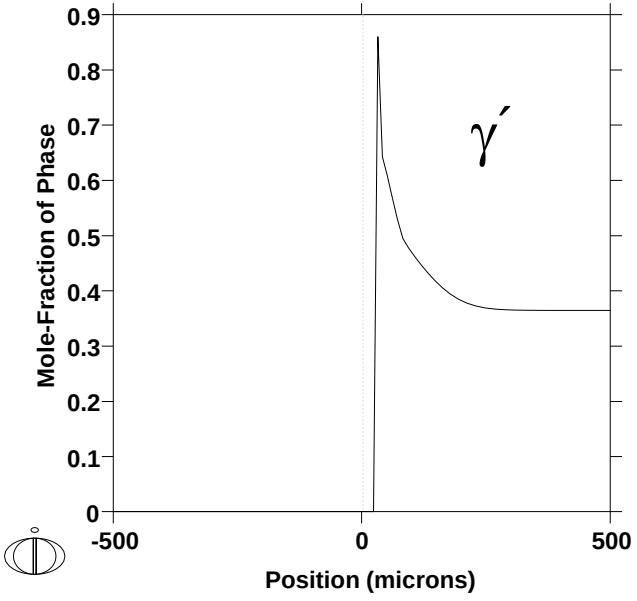
NiAl-coating / GTD111



Micrograph from E. Perez et al. J. Phase Equilib. Diffus., v. 27 (2006), pp. 659-664.

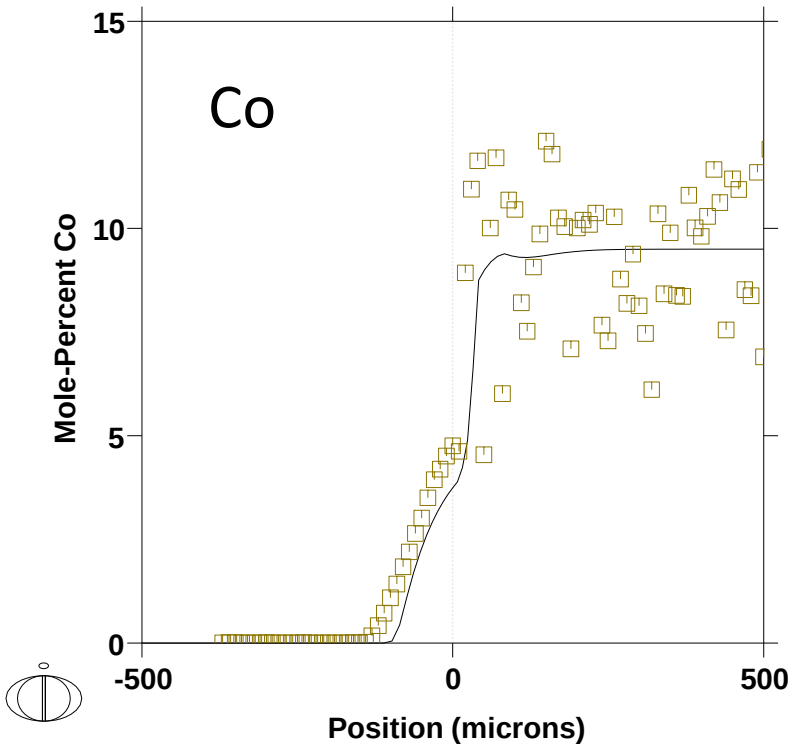


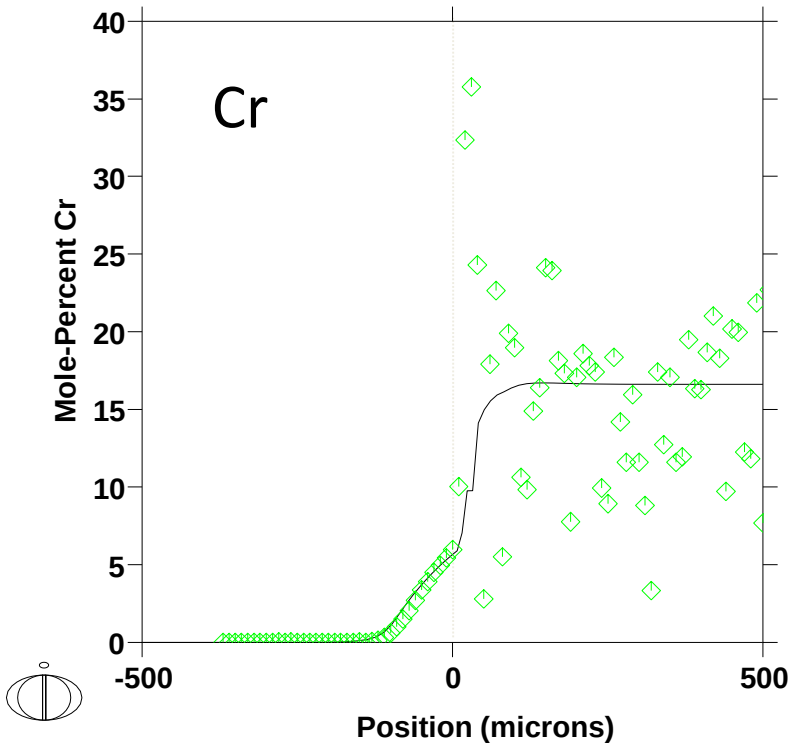




Engström et al., Advanced Materials Research Vol. 278 (2011) pp 198-203.

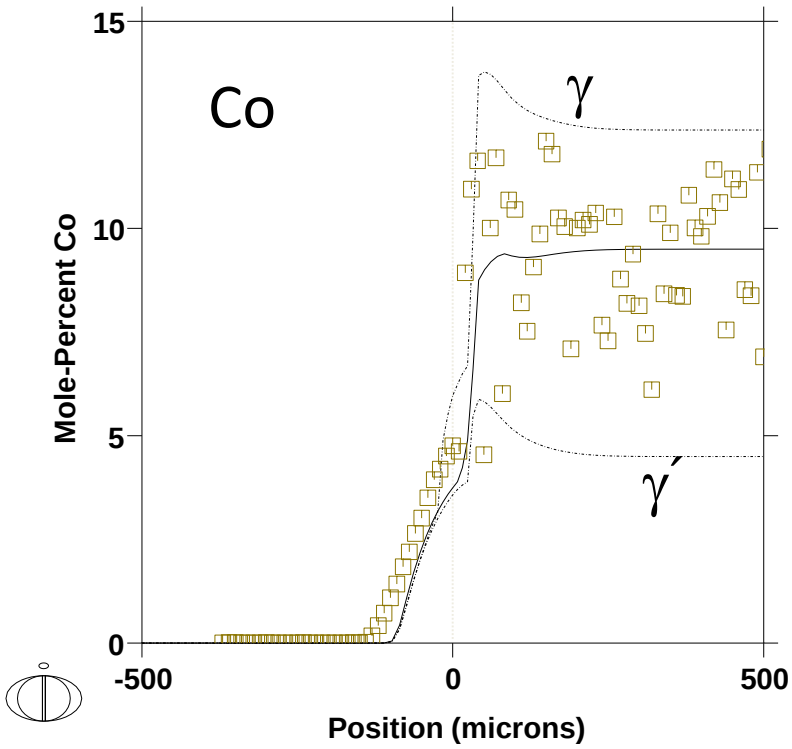
NiAl-coating / GTD111

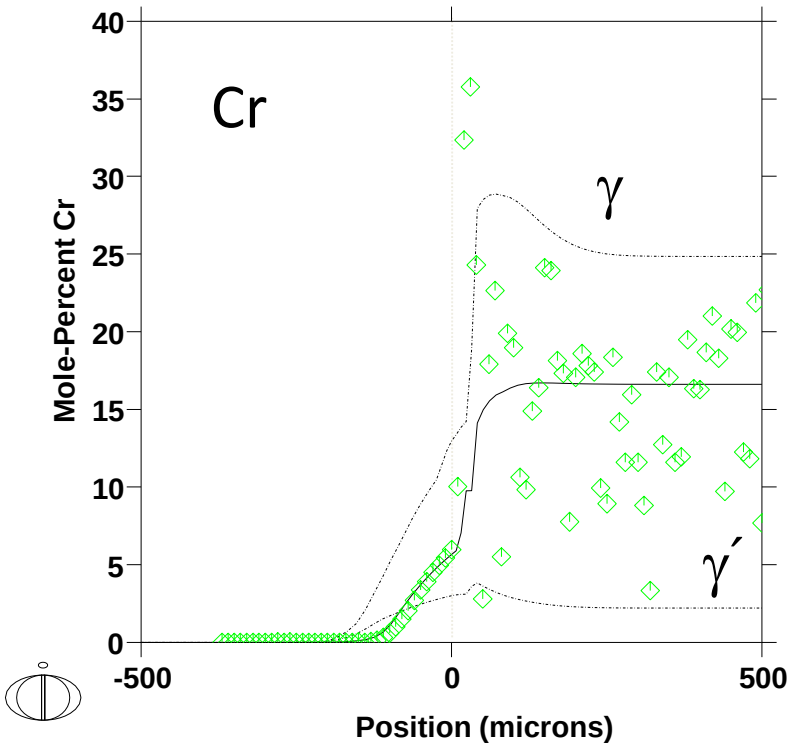




Engström et al., Advanced Materials Research Vol. 278 (2011) pp 198-203.

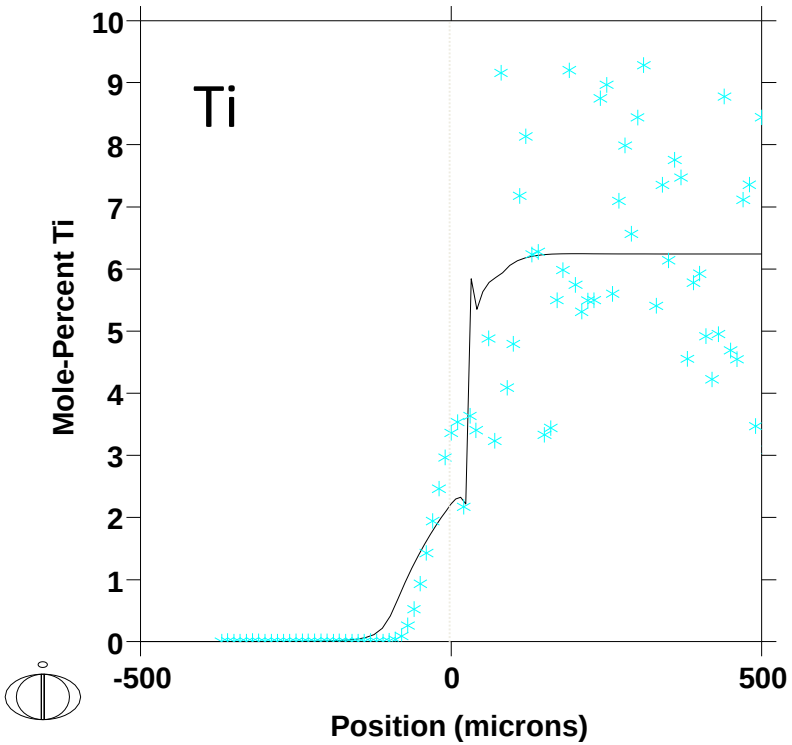
NiAl-coating / GTD111

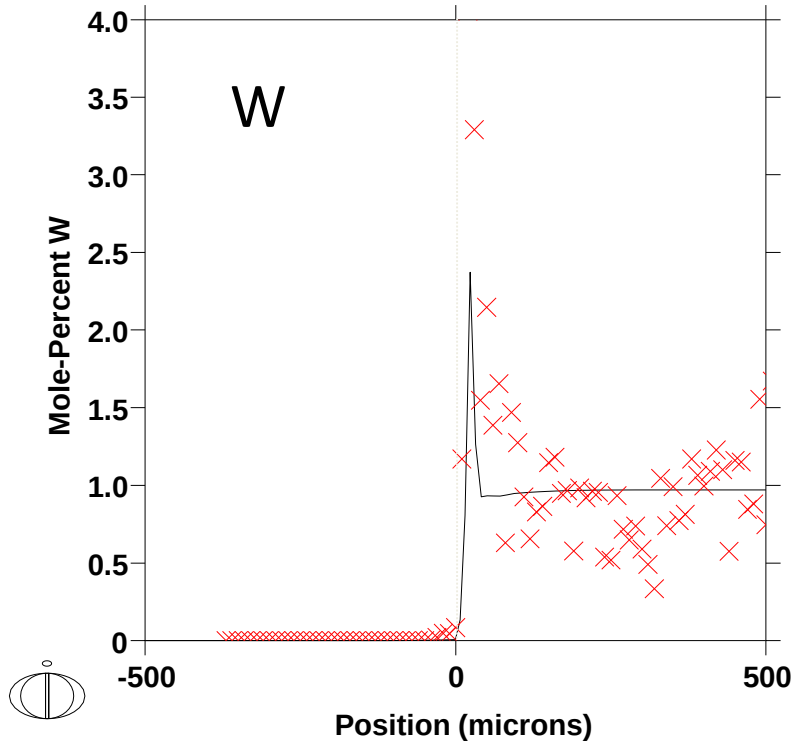




Engström et al., Advanced Materials Research Vol. 278 (2011) pp 198-203.

NiAl-coating / GTD111



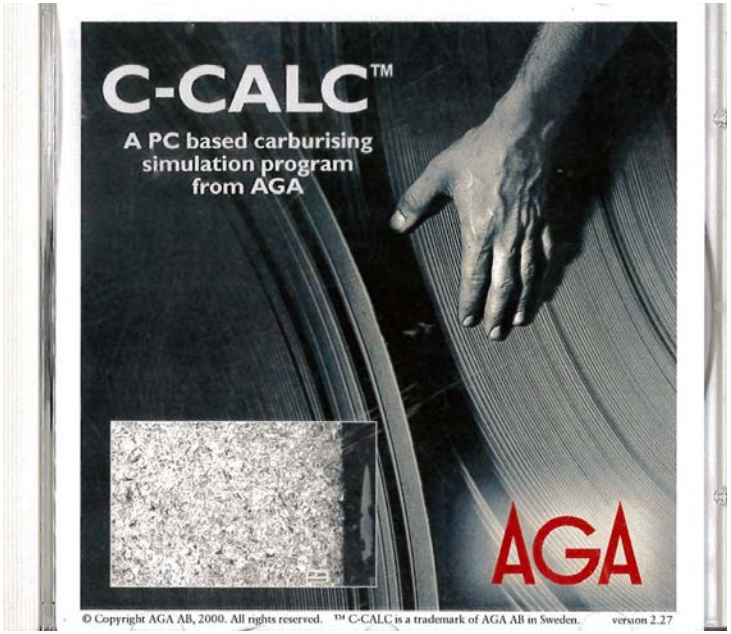


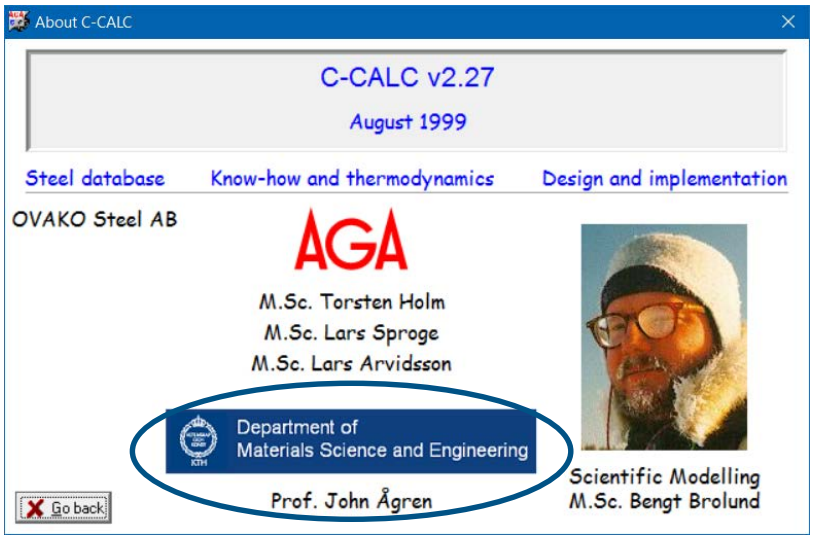
Engström et al., Advanced Materials Research Vol. 278 (2011) pp 198-203.

Outline

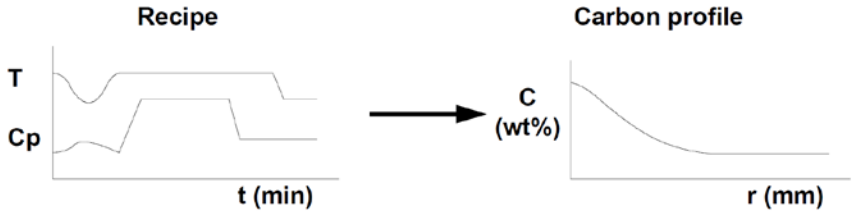
1. Introduction
2. Science
3. **Engineering**
4. Entrepreneurship

Simulation of case-hardening and control of furnace atmospheres

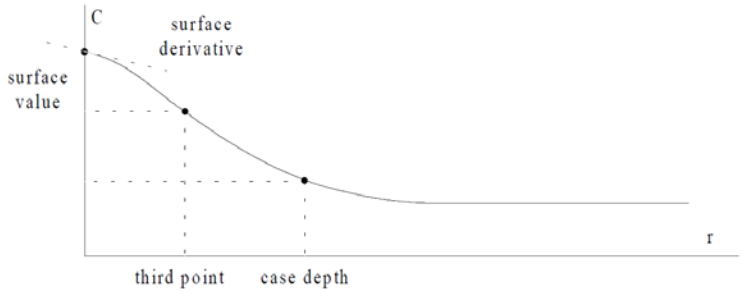




- Carburizing simulation tool



- Recipe design



Engineering solutions

Thermo-Calc Software

C-diffusion as function of composition and temperature:

$$D_c^{\gamma} = 4.53 \cdot 10^{-7}\left[1 + u_c(1-u_c)\frac{8339.9}{T}\right] \cdot$$

$$\exp\{-(1/T - 2.221 \cdot 10^{-4}) \cdot (17767 - 26436 \cdot u_c)\}$$

Ågren, *Scripta Metall., v* 20 (1986), p. 1507.

Influence from alloying elements:

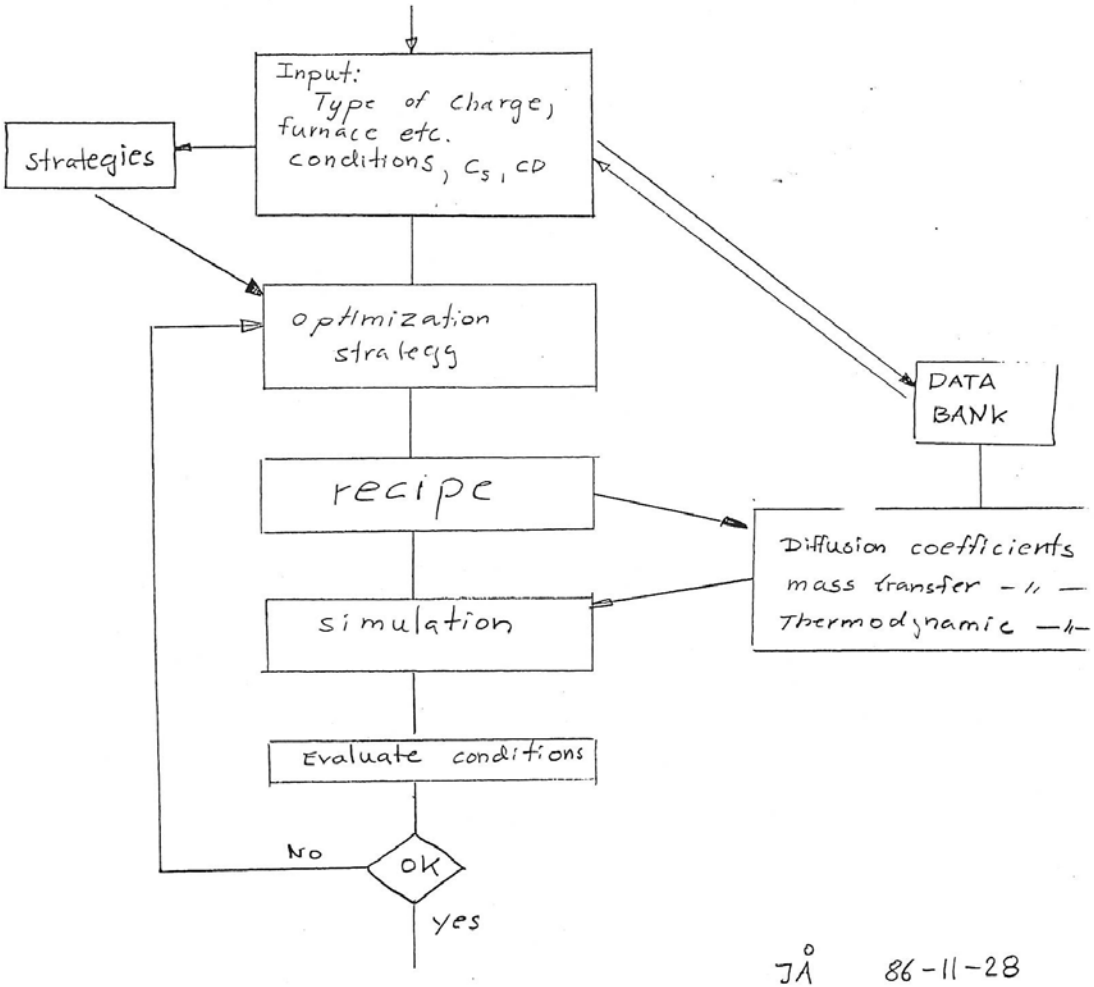
$$a_c = \frac{u_c}{1-u_c}\exp((5115.9 + 8339.9 \cdot u_c)/T - 1.9096) \cdot \exp(\sum k_M)$$

$$k_{Mn} = -(4810.9u_{Mn} + 1022u_{Mn}^2)/T$$
$$k_{Si} = 14793u_{Si}/T$$
$$k_{Cr} = (14.192 - 30207/T)u_{Cr}$$
$$k_{Ni} = 5532.5u_{Ni}/T$$
$$k_{Mo} = -10713.8u_{Mo}/T$$
$$k_V = -21649u_V/T$$

Ågren, Personal compilation, (1990).

Thermo-Calc Software

Recipe-Processing-Unit



JÅ 86-11-28

Outline

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2. Science
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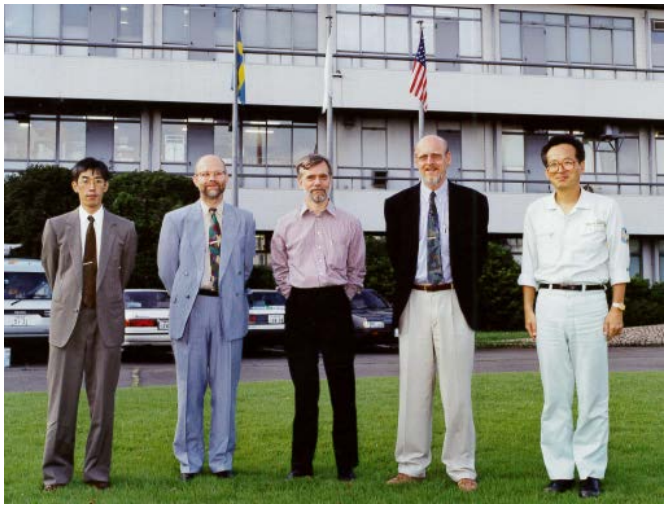
4. **Entrepreneurship**

Early dissemination (missionary)

- Driven by a desire to make research results come to use.



Visiting Nippon Steel in the late 80’s or early 90’s

Following the first training course in Japan about using the Diffusion Module (DICTRA).

Another foundation

- In 1993 John and six colleagues established a foundation. They donated their respective individual rights to the code for the benefit of this foundation.

- ***”Stiftelsen för Tillämpad Termodynamik”***

- This foundation became (and still is) the sole owner of all rights connected to the Thermo-Calc and DICTRA software.

- The purpose of the foundation is to support research in the field of computational thermodynamics.

- Today this is done in different ways, e.g. primarily by offering approximately $50K annually in travelling grants to young researchers.

Establishing Thermo-Calc Software AB

- In 1997 a company is created with the purpose of handling all administration, marketing, sales and support related to licensing of the Software.
- The foundation is the majority owner of the company with 80% of the shares, while the remaining 20% is controlled by the researches who had donated their individual rights for the benefit of the foundation.
- John has been on the Board of Directors since 1997, and served as Chairman of the Board since 2001.

Success by any measure

- Continuous growth

- 35 + 5 employees
- > 1250 customers in 60+ countries

- In a review of the 2015 literature, Thermo-Calc software products were referenced, mentioned or used in over 1000 publications, distributed on 231 journals, and by organizations from 59 different countries.
  - The topics range from the macro- to micro-level, from meteorites to platinum jewellery and power plants to nanowire systems.

and a new founding

Joint venture between QuesTek (US) and Thermo-Calc (Sweden)

- Founded in 2016, headquartered in Stockholm
- Building upon the success of QuesTek Innovations
  - Technical activities similar to QuesTek Innovations' but focused on the European market
- Business model: design, develop and patent new materials; license to producers/OEMs/end-users
- Offers materials design and modeling services
  - Design of novel advanced alloys
  - Optimization of existing alloys
  - Applying *Ferrium* steels to existing platforms

Congratulations to a real Superman

Thermo-Calc Software