Computational Thermodynamics and Kinetics

Seminar

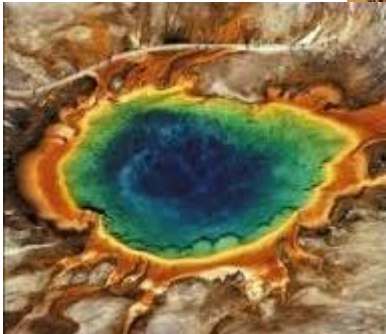*Stockholm, June 16, 2016*

Program

10.00 – 10.45   **News from Thermo-Calc Software: Thermo-Calc, DICTRA, TC-PRISMA and databases**
Dr. Johan Jeppsson and Dr. Qing Chen, Thermo-Calc Software

10.45 – 11.15   **Thermodynamic and Kinetic modelling – a Renaissance in materials science and engineering**
Prof. John Ågren, KTH, Sweden

11.15 – 11.30   Short break with fruits and water

11.30 – 11.50   **Calculating phase transformations in duplex stainless steels using computational thermodynamics**
Dr. Sten Wessman, KIMAB, Sweden

11.50 – 12.10   **Application of DICTRA in development of MCrAlX coatings**
Dr. Ru Lin Peng, Linköping University, Sweden

12.10 – 12.30   **Applications of computational thermodynamics in product and process development at SSAB**
MSc. Ulrika Borggren, SSAB, Sweden

12.30 – 13.45   Lunch

13.45 – 14.15   **Application of computational thermodynamics in materials industry**
Prof. André Costa e Silva, EEIMVR-UFF, Brazil

14.15 – 14.45   **Microstructure simulation in ICME settings**
Dr. Georg Schmitz, Access, Germany

14.45 – 15.15   **QuesTek Innovations' use of CALPHAD modelling and ICME for materials**
Dr. James Saal, QuesTek Innovations LLC, USA

15.15 – 15.45   Coffee break

15.45 – 16.05   **Solutions for metal cutting – applications of thermodynamic calculations**
Dr. Henrik Strandlund, Sandvik Coromant, Sweden

16.05 – 16.25   **Materials design from nano to macro based on ICME in Hero-m**
Prof. Annika Borgenstam, KTH, Sweden

16.25 – 16.45   **Towards an ICME methodology – Current activities in Europe**
Dr. Georg Schmitz, Access, Germany

16.45 – 17.00   **Open discussion**

Computational Thermodynamics

Making use of computer software and assessed thermodynamic databases to perform realistic calculations of thermodynamic properties of multi-component system.

A interdisciplinary science as thermodynamics is involved in many applied sciences.

CALPHAD

"CALPHAD (Computer Coupling of Phase Diagrams and Thermochemistry) aims to promote computational thermodynamics through development of models to represent thermodynamic properties for various phases which permit prediction of properties of multicomponent systems from those of binary and ternary subsystems, critical assessment of data and their incorporation into self-consistent databases, development of software to optimize and derive thermodynamic parameters and the development and use of databanks for calculations to improve understanding of various industrial and technological processes."

Source: www.calphad.org

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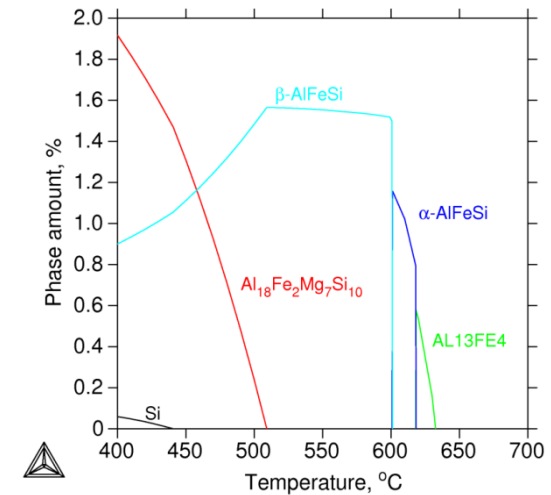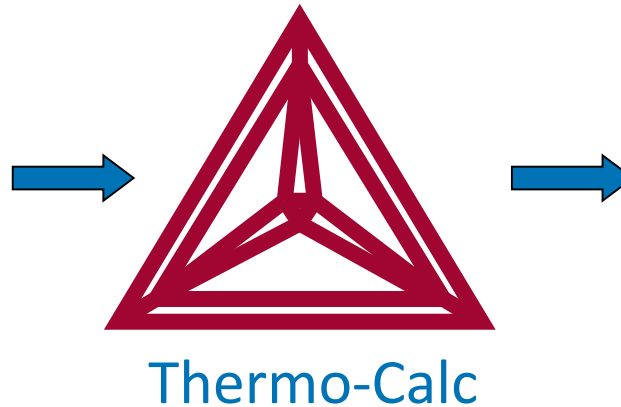"CALPHAD (Computer Coupling of Phase Diagrams and Thermochemistry) aims to promote computational thermodynamics through development of models to represent thermodynamic properties for various phases which permit prediction of properties of multicomponent systems from those of binary and ternary subsystems, <u>critical assessment of data and their incorporation into self-consistent databases</u>, development of software to optimize and derive thermodynamic parameters and the development and use of databanks for calculations to improve understanding of various industrial and technological processes."

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Thermo-Calc

Method

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

Early adoption

- In 1983, i.e. more than 30-years ago, SANDVIK, a global engineering group, had developed two new steels aided by CALPHAD-based calculations using Thermo-Calc.

- These two steels were SAF 2304 and SAF 2507 that later both became established grades.

25% Cr
7% Ni
4% Mo
0.3% Mn
0.3% Si
0.03% C
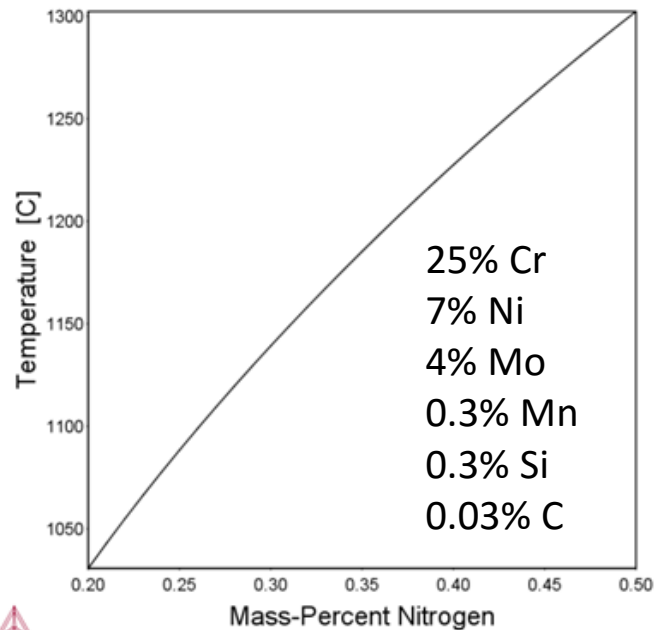
Calculation showing the temperature at which the fraction of ferrite equals 50%, as function of N-content.
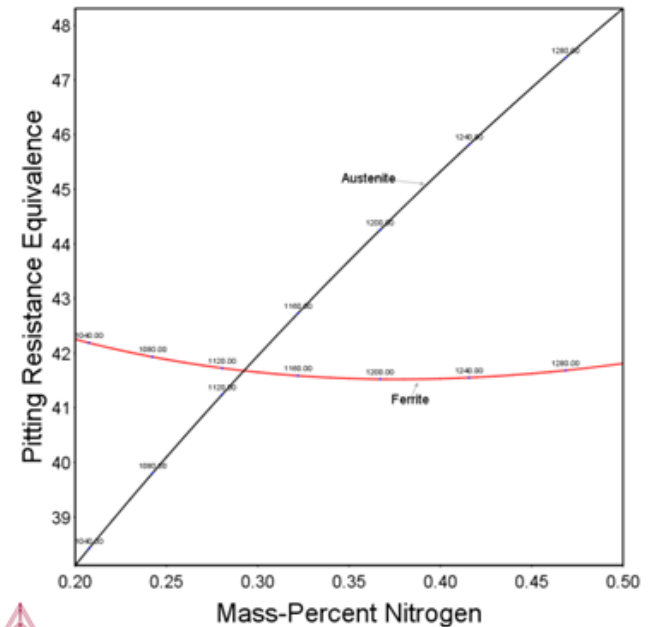
Calculated PRE for ferrite (red line) and austenite (black line), as function of N-content.

CALPHAD initially for representing thermochemical and phase-equilibrium information (the first materials genome) has proven extendable for other phase-based properties, e.g.

- Multicomponent diffusion kinetics
- Molar volume
- Viscosity
- Thermal and electrical conductivity
- Elastic constants
- Interfacial energy
- ...
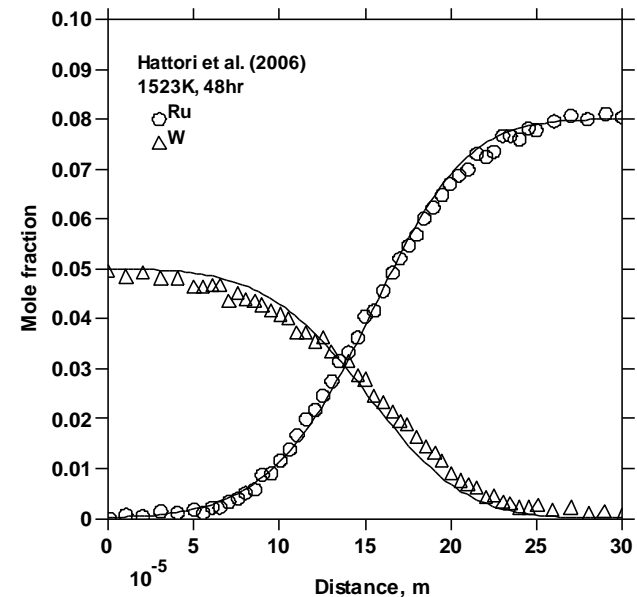
Allows us to apply ICME, as well as to simulate Process Structure Property relationships.

Booming usage

❑ 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.
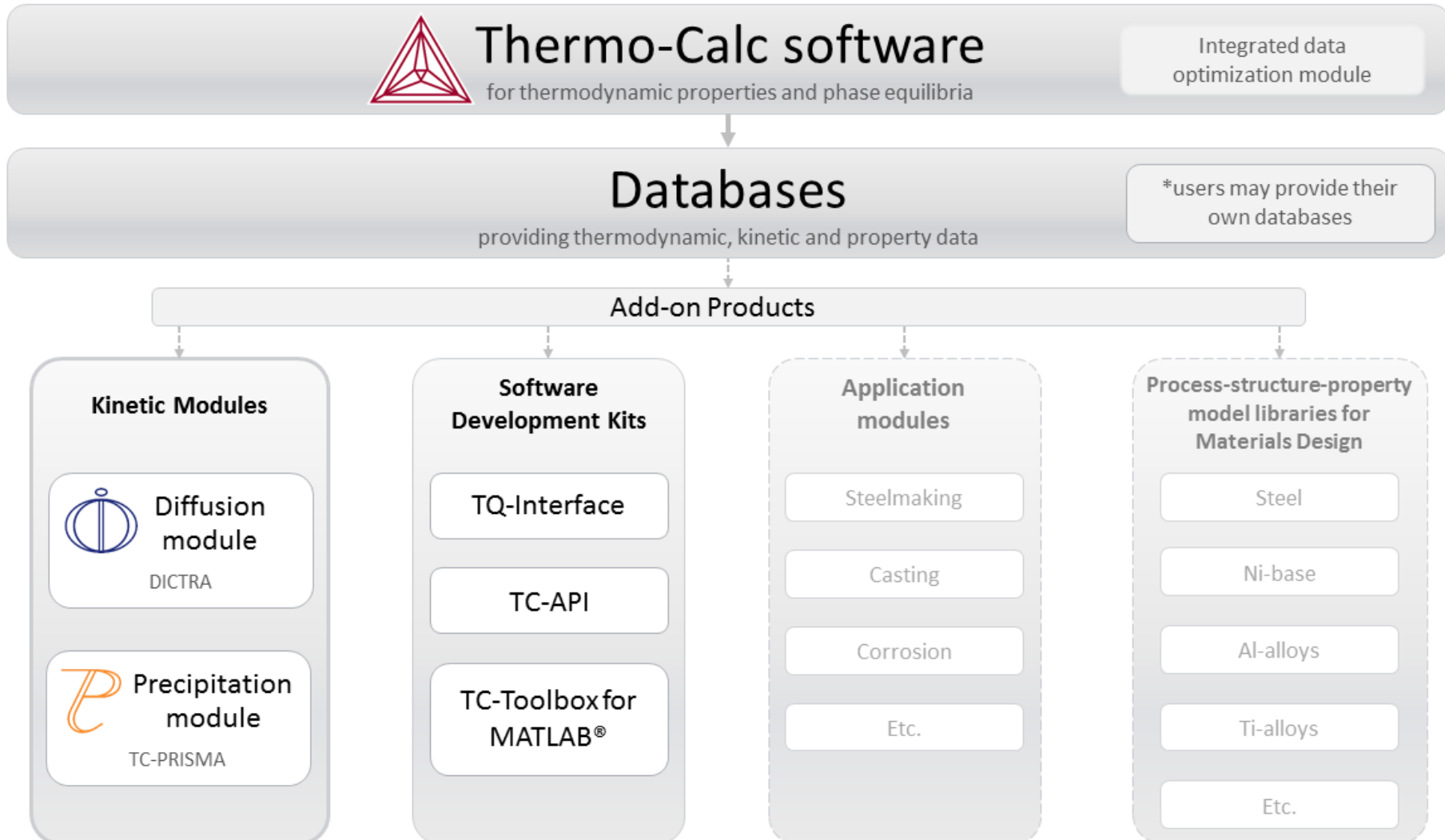
❑ 64 theses published in 16 countries.

   ❖ In 2015, at a minimum, sixty-four students, 64% at the PhD level, cited Thermo-Calc products.

❑ 46 patent citations (with a date of publication in 2015).

Product road-map

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