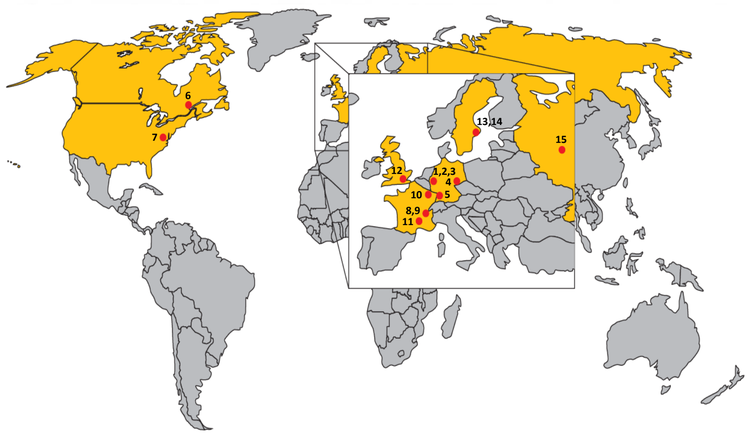
Scientific Group Thermodata Europe

A consortium of centers engaged in the development of thermodynamic databases for inorganic and metallurgical systems and their application to practical problems.

www.sgte.org

Chairman: T. Markus, Forschungszentrum Jülich, Germany



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SGTE is engaged in the critical assessment and compilation of thermodynamic data employing the CALPHAD method for inorganic and metallurgical substances, and has unique experience and expertise in the thermodynamic evaluation of data for solution phases.

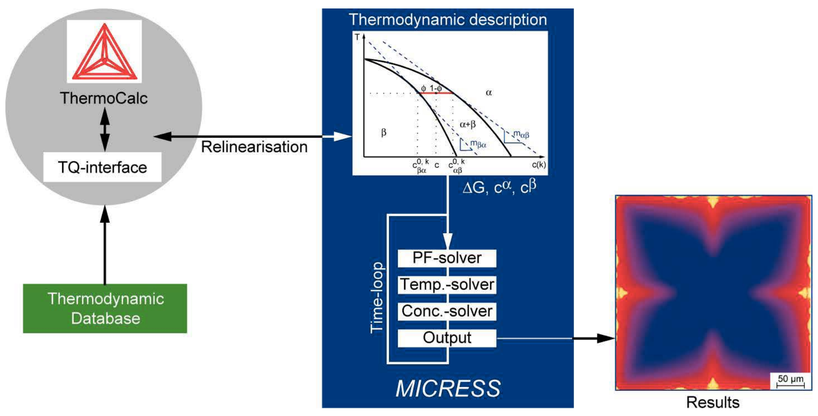
SGTE members help customers by providing consultancy services in the field of thermochemistry, holding workshops, and providing software packages including the **SGTE** databases. An organization that wishes to apply thermochemistry to solve practical problems, or to participate in workshops, should approach one of our members.

Application Examples from the SGTE *Casebook*

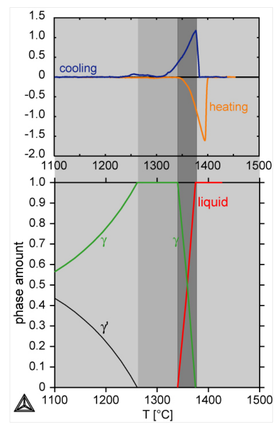
Microstructure of a five-component Ni-base superalloy: experiments and simulation

N. Warnken, B. Böttger, D. Ma, S.G. Fries, N. Dupin, B. Sundman

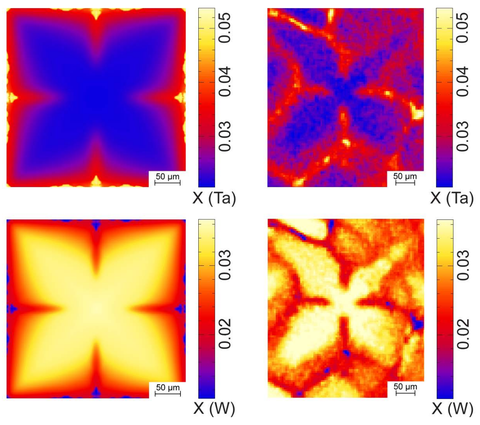
Coupling phase-field code with thermodynamic calculations is essential to realistically simulate microstructure evolution in multicomponent alloys. The authors simulated directional solidification modelling the isothermal dendritic cross-section. Results from thermodynamic calculations and the simulations were compared to results from experimental measurements of a five-component (Ni-Al-Cr-W-Ta) model superalloy. The constant cooling rate for the modelling was derived from experimental process parameters. Secondary phases were allowe to nucleate, their driving force for formation was calculated from the thermodynamic data.



Schematic representation of the approach for coupling the phase-field method with thermodynamic calculations.



DTA curves from heating and cooling at 5 K/min compared with calculated equilibrium phase evolution.

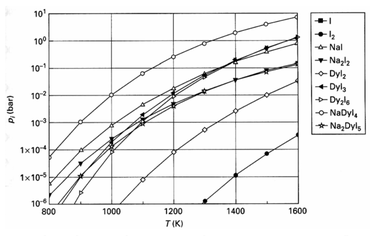


Simulated and measured elemental distribution maps scaled to the same range of 1.5 to 3.5 at.% for W and 2.1 to 5.3 at.% for Ta.

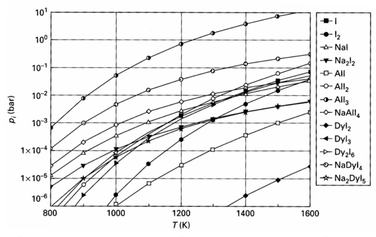
Relevance of thermodynamic key data for the development of high temperature gas discharge light sources

T. Markus, U. Niemann

An important variant of high-pressure Hg lamps are metal-halide lamps which are dosed with metal halides, e.g. NaI or DyI_3, to establish sufficiently large vapour pressures of the light emitting species. Because of the corrosive nature of the hot vapour polycrystalline Al_2O_3 is used as wall material to extend the lifetime of the lamp. Thermodynamic calculation of reactions among the lamp components provide important insight into the phenomena occurring during the operation of these lamps.



Calculated partial pressures of species in a 35 W lamp burner filled with DyI_3 and NaI.

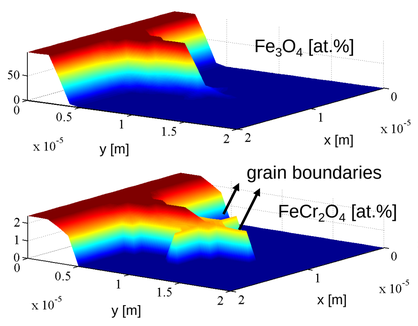


Calculated partial pressures in a 35 W lamp burner filled with DyI_3 and NaI with corrosion attack.

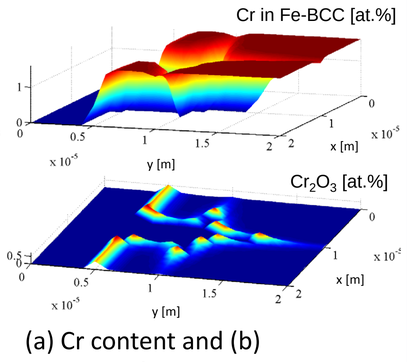
Thermodynamic modelling of processes during hot corrosion of heat exchanger components

U. Krupp, V. Braz de Trindade Filho, K. Hack

A model was used that is capable of simulating multiphase internal corrosion processes controlled by solid-state diffusion into the bulk metal as well as intergranular corrosion occurring in polycrystalline alloys owing to the fast inward transport of the corrosive species along the grain boundaries of the material. A finite-difference method was used to treat the internal corrosion problem.



The oxides in (a) the outer layer and (b) in the inner layer of a Fe-1.5 mass% Cr alloy.

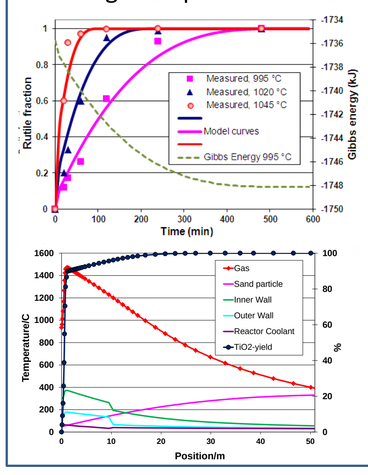


(a) Cr content and (b) intergranular Cr_2O_3 content in the surface zone of an Fe-1.5 mass% Cr alloy.

Modelling TiO_2 production by explicit use of reaction kinetics

P. Koukkari, R. Pajarre, K. Hack

Combined reaction rate – multiphase calculations were applied to two characteristic unit process of TiO_2 production: TiO_2 formation in a calciner and TiO_2 formation in a $TiCl_4$ burner. During the calcination process at relatively low temperatures a metastable form of TiO_2 , anatase, is formed first which is transformed into the stable rutile form in the high temperature zone of the furnace.



Anatase-rutile transformation kinetics in a Gibbs energy model at 995-1045 °C for the calcination process. The measured data are from McKenzie (Trans. J. Br. Ceram. Soc., 1975).

Calculated temperature and TiO_2 profiles. The O_2:$TiCl_4$ ratio was 1:1 and the initial mixing temperature was about 950 °C.

SGTE Products

SGTE Thermodynamic Databases

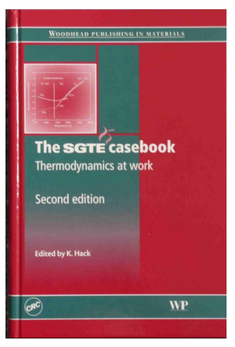
SGTE's core product are thermodynamic databases, which consist of assessed model parameters describing as accurately as possible experimental data on binary, ternary systems and higher order systems. The models are based on physical principles enabling extrapolation to commercial multi-component systems. However, extrapolation from several assessed lower order systems requires that these systems are internally consistent. A number of commercially interesting as well as scientifically challenging materials have been collected into databases which are listed below. Most of these are available for a fee. **SGTE** Databases are under continuous development:

- **UNARY** — Assessed thermochemical data for all stable and many metastable modifications from 298.15 K up to the gaseous state for 83 elements. It is freely available.
- **SGSUB** — The Substance Database contains thermochemical data for about 4300 condensed or gaseous species in the standard state.
- **SGSOL** — The Solution Database contains data for the liquid phase and various crystalline phases of the pure elements in addition to over 700 binary, ternary and quaternary alloy systems and more than 1300 intermediate phases.
- **SALT** — This molten salt database originates from FACT, Montreal, Canada, and has been modified by Alan Dinsdale, NPL, and adopted by **SGTE** in May 1993.
- **SLAG** — Database from IRSID / Arcelor Research for Fe-containing slags consisting of data for the liquid slag and condensed oxides for the Al_2O_3-CaO-FeO-Fe_2O_3-MgO-SiO_2 system and 25 trace components. Recently, data for Na, Cr, Ni, P and S have been added.
- **SEMICONDUCTOR** — This database contains all 15 binary systems between the group III elements Al, Ga and In and the group V elements P, As and Sb. It is freely available.
- **NOBLE Metals** — The noble metal alloy database originates from a collaboration between the Spencer Group and GTT-Technologies. It is based on 8 noble metals with addition of 22 alloying elements.
- **NUCLEAR** — The database has been generated by THERMODATA and is specially made for the investigation of in-vessel chemical reactions.
- **Thermal Barrier Coating (TBC)** — The database consists of four separate sets describing thermodynamic parameters for the ZrO_2-RE_2O_3-Y_2O_3-Al_2O_3 systems (RE=Gd, Sm, Nd, La) for calculation of phase relations between top coat and thermally grown oxide (Al_2O_3).

ThermDoc / Papyrus

ThermDoc is a bibliographic database of scientific journal articles covering thermodynamics of inorganic systems and is developed by **SGTE** members and updated twice a year.

Papyrus is the corresponding database management software offering flexible and sophisticated means of retrieving references. Efficient and easy to use, one can also create and manage own bibliographic databases. In 2008 more than 79.000 records were available in ThermDoc and about 2000 new references added each year. The software package is available for Windows®. Each record in the database consists of : Title, Authors' names, Complete bibliographic reference.



The SGTE casebook - Thermodynamics at work

edited by K. Hack, 2nd edition, 2008

Woodhead Publishing: ISBN 978-1-84569-215-5; CRC Press: ISBN 978-1-4200-4458-4

The ***casebook*** presents the theoretical background to thermodynamic modelling and its wide range of practical applications. These applications include the analysis of various types of high-temperature corrosion, understanding the loss of corrosion resistance in steels, the processing of steels, as well as the use of thermodynamics to improve the functionality of materials for microelectronics and lighting applications, and in the analysis of nuclear safety issues.

Applications to kinetically-controlled processes such as the solidification, melting and heat treatment of alloys and production of silicon and titanium oxide pigment are also illustrated.

The **SGTE** casebook is a valuable reference for those manufacturing steels and other materials, those using materials in high-temperature applications such as the power industry and also those engaged in other areas such as microelectronics and lighting.

Thermodynamic Properties of Inorganic Materials – Landolt-Börnstein Group IV (Physical Chemistry), volume 19

Springer ISBN: 3540653279

This book series provides calculated thermodynamic data using **SGTE** databases for inorganic substances and mixed system. in mixed systems all solid solutions having the same crystal structure are represented by a common phase model.

The **SGTE** evaluated data are presented in 3 subvolumes:

A: Pure Substances — Standard thermodynamic properties for each substance, together with plotted heat capacity, Gibbs energy and enthalpy of formation functions up to the maximum temperature for which the data for that substance have been evaluated.

B: Binary Systems — Phase diagrams, phase transition data, integral and partial quantities of alloys .

C: Ternary Steel Systems — Liquidus and solidus projections, isothermal section, isopleths, reaction schemes.