Scientific Group Thermodata Europe

Torsten Markus

Scientific Group Thermodata Europe (SGTE), 6 rue du tour de l'eau, 38400 St Maintint d'Heres, France

info@sgte.net

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.net

Chairman: T. Markus, Hochschule Mannheim, Germany

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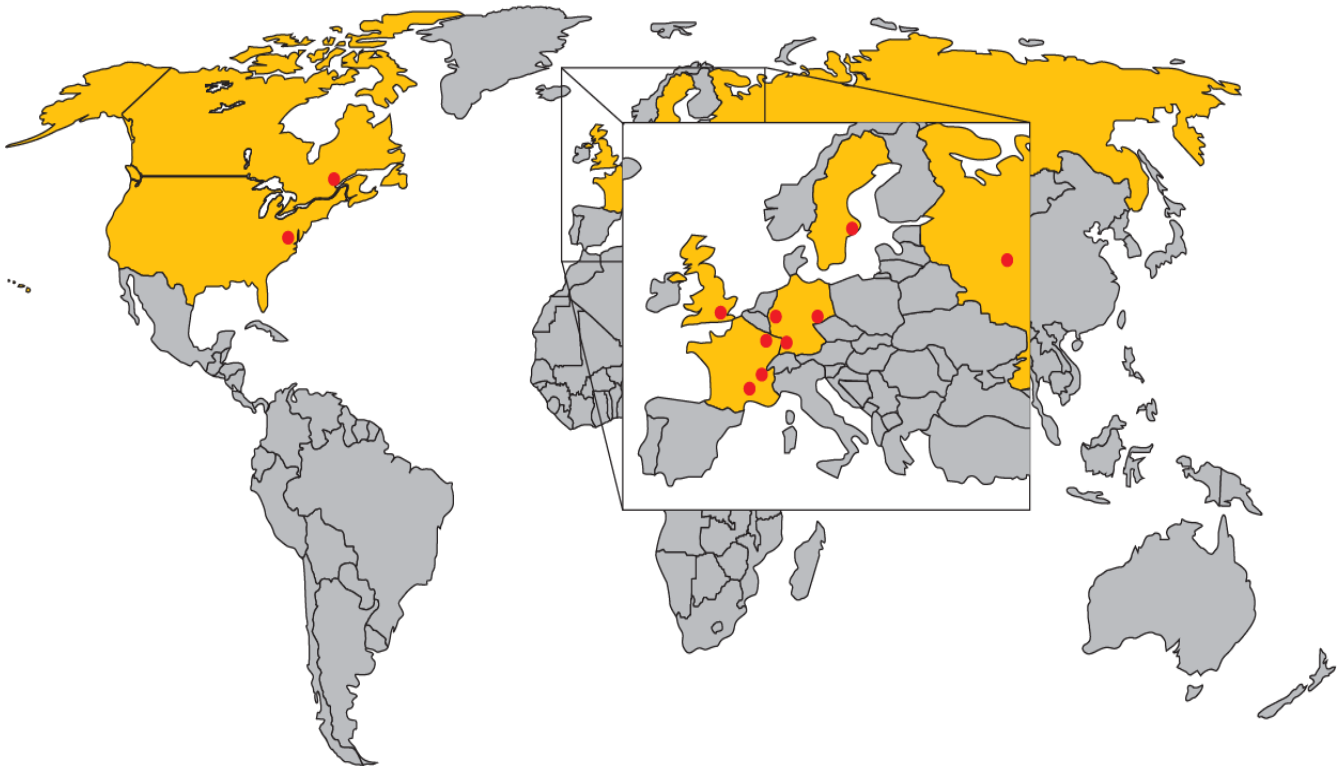


GERMANY
(1) RWTH Aachen University, Aachen
(2) GTT Technologies, Herzogenrath
(3) Forschungszentrum Jülich GmbH, Institute for Energy Research (IEF-2), Jülich
(4) The University of Freiberg, Freiberg
(5) Karlsruhe Institute of Technology (KIT), Karlsruhe

CANADA
(6) Thermfact, Montréal

USA
(7) National Institute of Standards and Technology (NIST), Gaithersburg, MD

FRANCE
(8) THERMODATA, Grenoble
(9) Institut National Polytechnique de Grenoble (LTPCM)
(10) Arcelor Research, Maizières-les-Metz
(11) The University of Montpellier 2, Montpellier

GREAT BRITAIN
(12) National Physical Laboratory, Teddington

SWEDEN
(13) KTH Royal Institute of Technology, Stockholm
(14) Thermo-Calc Software, Stockholm

RUSSIA
(15) Glushko Thermcenter of the Russian Academy of Sciences, Moscow
(16) MISIS, Moscow

Scientific Group Thermodata Europe

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.

- SGTE is at the forefront of providing critically assessed thermodynamic data for alloys
- Use of the expertise of SGTE members in inorganic chemistry and materials science
- Development of standard reference data for the elements - used worldwide
- Promotion of guidelines for modelling of data for phases
- Development of self-consistent and inter-consistent databases
- Use of well-defined quality procedures
- Promotion of workshops to explore future needs and developments

Software developed by SGTE Members

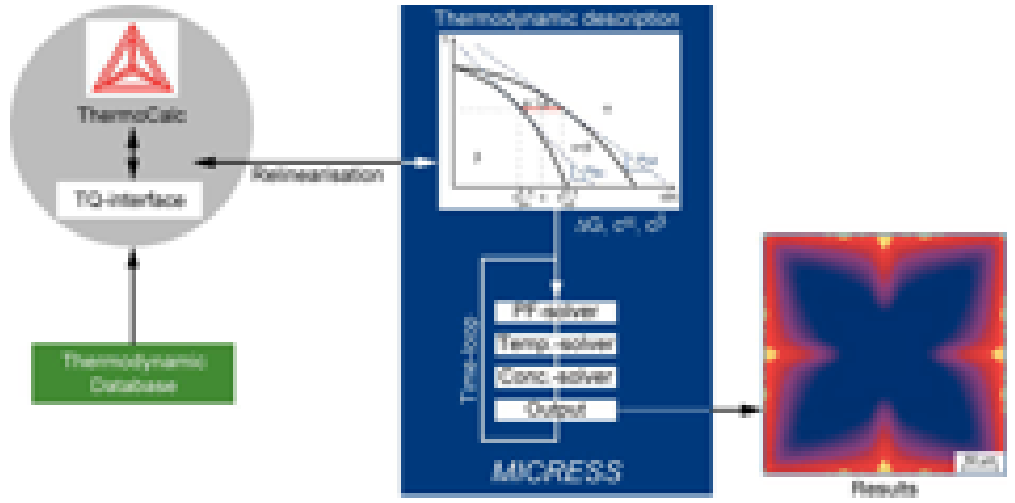
- MTDATA
- ThermoCalc
- FactSage (FACT & ChemSage)
- COACH & GEMINI
- BINGSS etc..

Application Examples from the SGTE *Casebook* 1

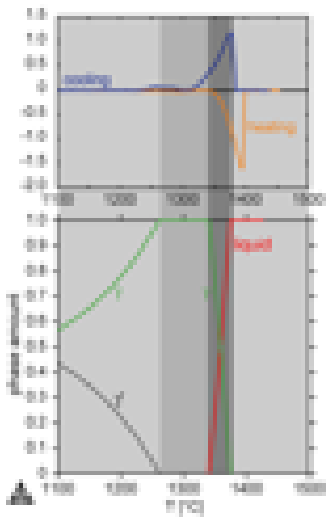
Microstructure of a five-component Ni-base superalloy: experiments and simulation

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

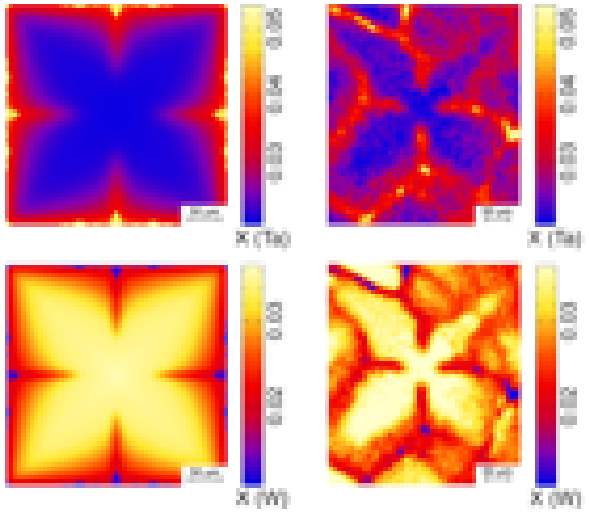
Coupling phase-field code with thermodynamic calculations is essential to realistically simulate microstructure evolution in multicomponent alloys. The authors simulated directional solidification modelling the isothermal dendritic cross-section. Results from thermodynamic calculations and the simulations 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.



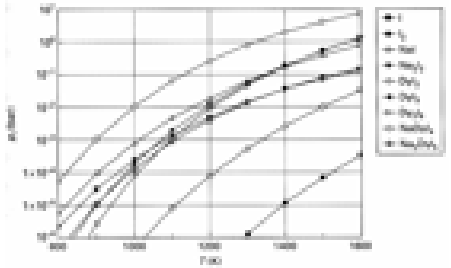
Simulated and measured elemental distribution maps scaled to the same range of 1.5 to 3.5 at.% for W and 2.1 to 5.3 at.% for Ta.

Application Examples from the SGTE Casebook 2 + 3

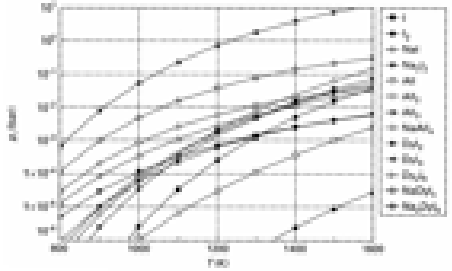
Relevance of thermodynamic key data for the development of high temperature gas discharge light sources

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.

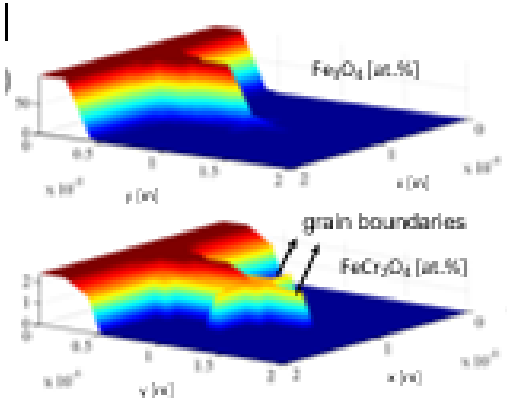


Calculated partial pressures in a 35 W lamp burner filled with DyI_3 and NaI with corrosion attack.

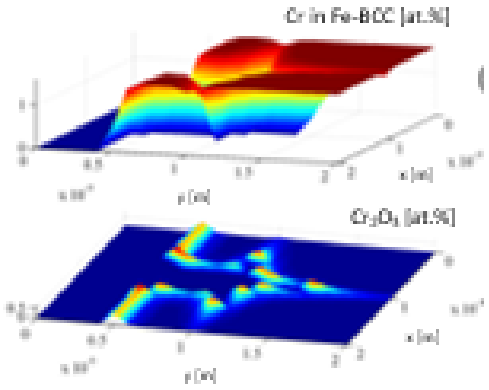
Thermodynamic modelling of processes during hot corrosion of heat exchanger components

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.

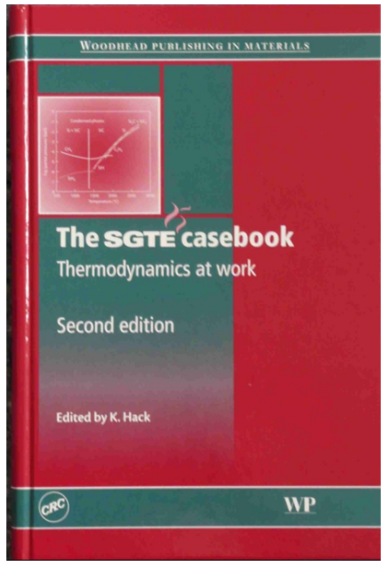
SGTE Products

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).

SGTE Products



The SGTE casebook - Thermodynamics at work

edited by K. Hack, 2nd edition, 2008

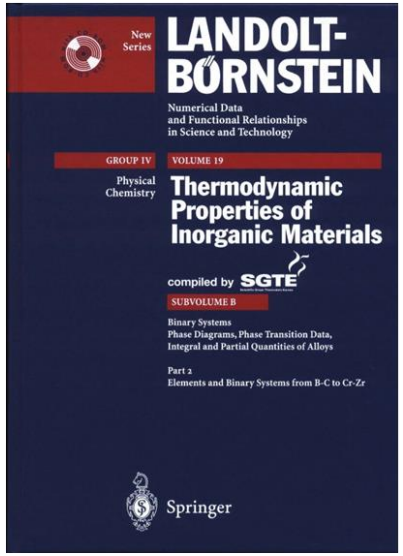
Woodhead Publishing: ISBN 978-1-84569-215-5; CRC Press: ISBN 978-1-4200-4458-4

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.

SGTE Products



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.

SGTE Products

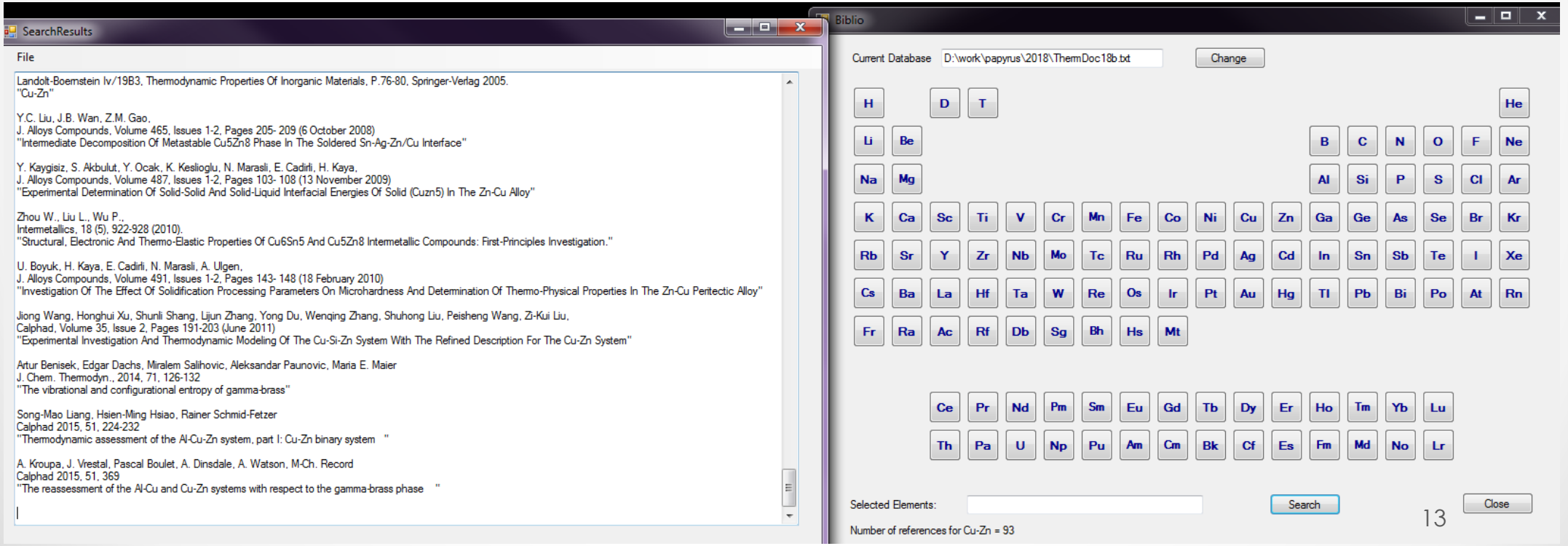
ThermDoc / Papyrus

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.

ThermDoc

- Collection of references compiled by SGTE
- Current database contains over 90000 references
- Searchable by system name
- Coverage is general but not complete
- Available at no cost



New data for the elements

- Most of the element data derived 25+ years ago – served us well !
- International collaboration underway to carry out a complete reassessment of data for the elements supplemented by new experimental work and ab initio calculations
  - KTH, TCSAB, Hampton Thermodynamics, MISiS, TCRAS, NIST, MPI Dusseldorf
- Aim is to use physically realistic models selected at Ringberg meeting in 1995:
  - Einstein model or similar for crystalline phases down to 0 K with correction
  - Two state model for the liquid phase to provide a sound basis for extrapolating the heat capacity to temperatures below the melting point
  - data for the gas phase in terms of molecular constants and electronic energy levels
- Allow more reliable extrapolations beyond regions of stability
  - Liquid below melting point
  - Crystalline phases above melting point
- Elements being covered include:
  - Fe, Cr, Mn, Ni, C, Co, Al, Zn, Cd, Sn, Pb, Bi, In, Sb, Ag, Cu, Ge, Si, Au, Li, Na, K, Rb, Cs, Hg

Thank you for your attention

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