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A brief history of CALPHAD

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Abstract

Some 35 years ago, Larry Kaufman and Himo Ansara provided the stimulus to bring together a small number of scientists who were working on the calculation of alloy phase diagrams using as basis the required consistency of experimental thermodynamic and phase boundary data. This group represented the origins of CALPHAD and of subsequent developments concerned with computer coupling of phase diagrams and thermochemistry. From those origins, the "CALPHAD Method" has become a successful and widely applied tool in all areas of materials development.

The present paper presents a brief account of the development of CALPHAD, with particular emphasis on the earliest years of its formation and growth.

Keywords: CALPHAD; Thermodynamics; Phase diagrams

1. Introduction

For over 30 years now, an international group of scientists has been working closely together to develop methods, and to produce data, which provide a mutually consistent description of the thermodynamic properties and phase diagrams of materials systems. The group is known by the name CALPHAD (**CAL**culation of **PHA**se **D**iagrams) and the methodology it uses has become sufficiently well known, that the approach is referred to in the scientific literature as "The CALPHAD Method".

Since the early 1970s, the lively interactions between scientists participating in CALPHAD meetings and contributing to the CALPHAD journal [1] have been a major factor in the very rapid advances taking place in the field of computational thermochemistry.

In the earliest days of computer growth, a pre-CALPHAD group of scientists was busy performing what are now considered to be "simple" phase diagram calculations by feeding computers, which occupied whole rooms or even floors of large buildings, with punched cards and paper tape.

From those beginnings, and with ever-increasing sophistication of the computers and the science, the CALPHAD approach to phase diagram computation has increased both in terms of the number of scientists engaged in the work and the types of materials and problems to which the CALPHAD method is being applied. A core activity throughout the years has been the development and testing of models to describe the thermodynamic properties of different types of phase, as well as the reliable extrapolation of those properties from binary to ternary and higher-order systems. This has led to the development of powerful software for the critical evaluation of thermochemical data, by means of which compatibility of experimentally determined thermodynamic properties and phase boundaries of a system is assured. Further developments in software and data have resulted in the availability of commercial packages (also developed by scientists within the CALPHAD tradition) for calculation of complex chemical equilibria. Such packages are contributing to the present wide use of computational thermochemistry as a basic tool in materials production and processing.

The CALPHAD achievements in this field are due, in no small measure, to the enthusiastic and inspiring leadership of Larry Kaufman, to the equally strong support of the late Himo Ansara and to the efforts of the international group of scientists who have remained dedicated to this particular field of science, and to the support of each other's work, over many years.

Many aspects of computational thermochemistry, including the techniques used in carrying out thermodynamic assessment

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work, and the use of First Principle methods to obtain missing thermodynamic values and even calculate complete phase diagrams, are now well established. It is of particular interest, therefore, to look back to the early years of CALPHAD to trace how the present capabilities have developed from very humble origins.

2. Origins of CALPHAD

Although the relations between the various thermodynamic functions and the equilibrium phase diagram of a binary system had already been described in detail by Van Laar in 1908 [2], it was only with an increasing accumulation and accuracy of experimental thermodynamic data, that more attention was given to the evaluation of phase boundaries in alloy systems by use of thermodynamic calculations. Wagner [3] discussed a number of features of equilibrium diagrams and their relation to Gibbs energy, enthalpy and entropy values, and Meijering summarized earlier work on the construction of equilibrium diagrams using thermochemical data [4].

In these earlier years of the subject, before the advent of the computer, or even the desk calculator, phase diagrams were, of necessity, derived by constructing common tangents to hand-calculated Gibbs energy curves, using a ruler. This approach to the use of thermodynamic data in constructing phase diagrams is best summarized in a paper by Kubaschewski and Chart [5], in which the thermodynamic assessment, including "hand construction", of several different types of phase diagram is described.

A major advance in the capability for wider use of thermodynamic phase diagram calculation techniques was provided by Kaufman, who illustrated the importance and use of the concept of "lattice stabilities" in calculating phase diagrams. Lattice stability values, the differences in Gibbs energy between different stable and metastable crystallographic forms of an element as a function of temperature, allowed the equilibrium boundaries between the different phases of a system to be calculated more accurately. The concept of lattice stabilities, and some calculated phase diagrams, are presented in Ref. [6], while an extensive set of data for the Gibbs energy differences between the fcc, bcc and hcp structures of a large number of elements is provided in Ref. [7]. Fig. 1 presents enthalpy and entropy differences between the hcp and bcc forms of transition metals used by Kaufman in 1970 [7].

In 1968, Hillert [8] described in some detail the significant advances in phase equilibrium studies that could be achieved if experimental thermodynamic and phase diagram data were combined using computer techniques and the resulting assessed values employed universally.

The first scientific meetings to include sessions on computer calculation of phase diagrams were those concerned with the general topic of metallurgical chemistry held in Münster, Germany, at Brunel University and the National Physical Laboratory, UK, in 1971, and it was these meetings that resulted in the initiative to establish a working group concerned with the computer calculation of phase diagrams. This began in 1973 as a joint proposal by Larry Kaufman of ManLabs in Boston, USA and Himo Ansara of the University of Grenoble, France, that centres involved in such activities be invited to take part in two meetings, to be held at ManLabs, and the University of Grenoble. The aim of the proposed meetings was first to exchange ideas and discuss specific problems associated with the work, but also, if possible, to coordinate the activities being carried out in different laboratories on the thermodynamic assessment of alloy phase diagrams. The content of the letter they sent out to potential participants in such an activity included the following:

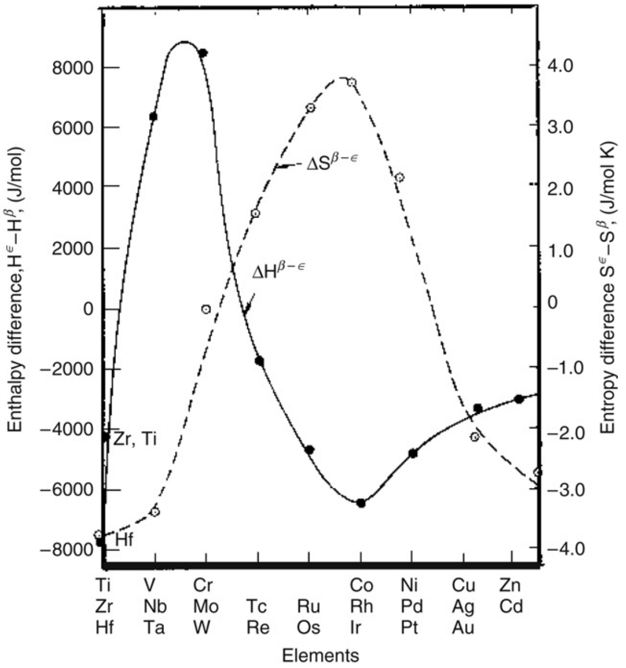

Fig. 1. Enthalpy and entropy differences between the hcp and bcc forms of transition metals [6].

We believe that substantial progress can be made in a short period of time if we could arrange to work together for one week at one of our facilities to define problems, disband, carry out some individual activities and meet again for a week at a second facility to compare results and chart future activities.

At that time, such calculations were in their infancy, and apart from Kaufman's group at ManLabs, only three European groups had thermodynamic calculation of phase diagrams as a major research theme. The groups concerned were located at the University of Grenoble, France (led by I. Ansara), the Royal Institute of Technolgy, Stockholm, Sweden (led by M. Hillert) and at the National Physical Laboratory, Teddington, UK (led by O. Kubaschewski).

The first CALPHAD meeting was organized and hosted by Larry Kaufman at ManLabs in Boston. It was held from 5–9 November 1973. To accommodate those attending the meeting, Larry reserved three double rooms and one single room at the Fenway Cambridge Motor Hotel (at a charge of \$20 per night for the single room and \$29 per night for the double rooms). The scientists invited to attend were Himo Ansara and Claude Bernard from LTPCM, ENSEEG, Grenoble, France, Oswald Kubaschewski (then having moved from the UK to Germany) and Ihsan Barin from RWTH Aachen, Germany,

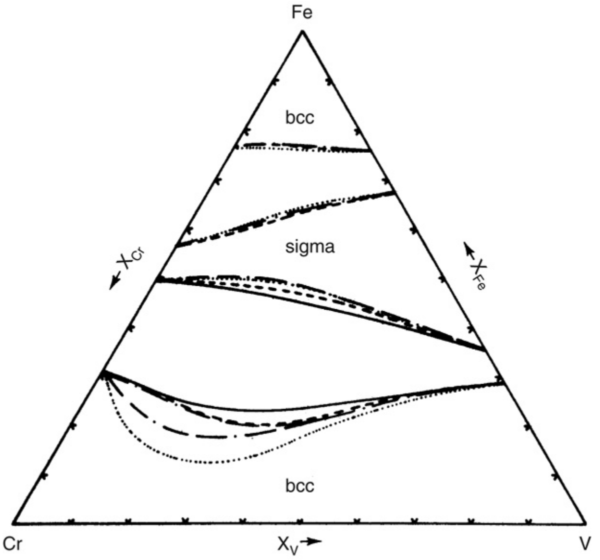

Fig. 2a. Isothermal section of the Fe–Cr–V system at 973 K calculated using different interaction models.

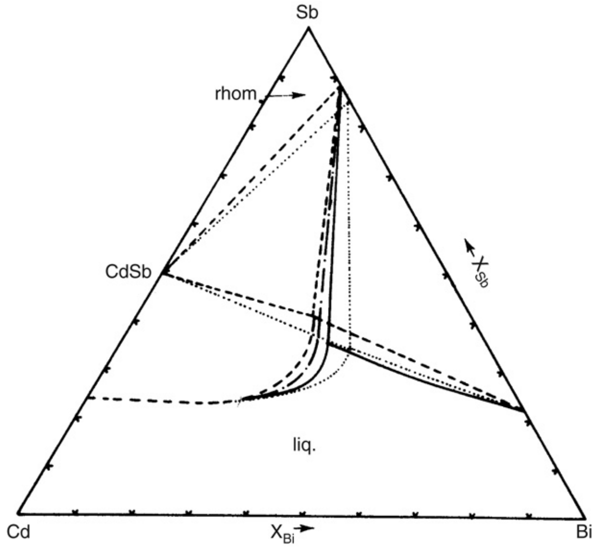

Fig. 2b. Isothermal section of the Cd–Bi–Sb system at 643 K calculated using different interaction models.

Philip Spencer and Jack Counsell from NPL, Teddington, UK, and Mats Hillert and Gernot Kirchner from KTH, Stockholm, Sweden. Apart from Larry Kaufman, others attending from the USA were Harvey Nesor from ManLabs, John Cahn (then at MIT), Dick Weiss from AMMRC Watertown, and Claude Lupis from Carnegie Mellon University in Pittsburgh.

The meeting was both stimulating and exhausting, with all sessions taking place in a windowless room to promote concentrated discussion! Lunch bags provided the only slight distraction from the continuous scientific exchanges. As Ihsan Barin put it later — "it was a little like one might imagine a thieves' kitchen to be, but in this case with calculated phase diagrams being pushed around the table and three or four binaries being offered for one ternary".

3. Discussion topics at CALPHAD 1

Below is a summary of the topics discussed, together with the conclusions drawn. The latter are presented here as reported.

Pure elements — It was suggested that periodic re-evaluation of the lattice stabilities of metals such as Mn and Fe should be made. Further, attention should be given to the role of the specific heat of the liquid phase in defining the free energy differences between liquid and solid over a wide temperature range. In particular, the linear term in the high temperature specific heat should be analysed.

Binary systems — The phase diagrams of the Cd–Sb, Cr–Fe, Ti–Ni, Bi–Sb and Cr–Co systems were calculated from given sets of thermodynamic properties of mixing by three independent centers, using either the equality of chemical potentials or the minimization of the free energy of the system. The results showed that, at this stage, the calculated phase diagrams are in good agreement.

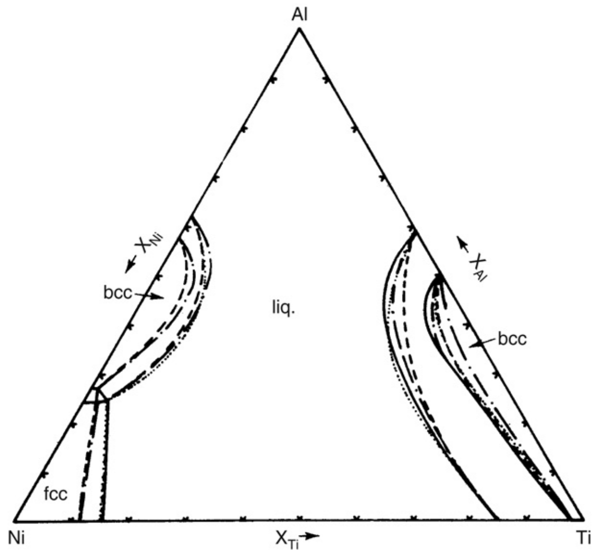

Fig. 3a. Isothermal section of the Al–Ni–Ti system at 1600 K calculated using the Kohler and Toop "interaction models".

Ternary systems — The Cd–Sb–Bi, Al–Ni–Ti and Fe–Cr–V phase diagrams were calculated using binary data and different interaction models. Results obtained for the Cd–Sb–Bi and Fe–Cr–V systems showed surprisingly good agreement when using the Margules, Kohler and Toop equations (see Figs. 2a and 2b taken from Ref. [9]). However, there were differences between the phase diagram of the Al–Ni–Ti system as calculated using the Margules equation on the one hand and the Kohler and Toop equations on the other (see Figs. 3a and 3b taken from Ref. [9]).

Analysis of interaction models: substitutional and interstitial solutions — As indicated in the previous topic, different interaction models can lead to significantly different results. For the cases considered, the Margules equation tends to lead to lower thermodynamic properties of mixing than those obtained

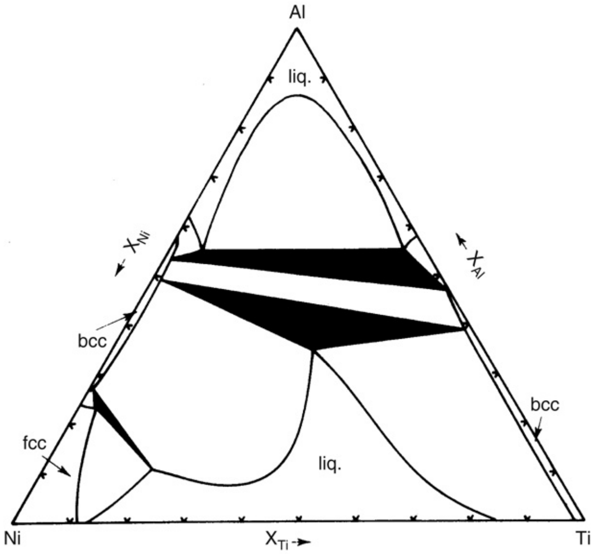

Fig. 3b. Isothermal section of the Al–Ni–Ti system at 1600 K calculated using a Margules-type “interaction model”.

using the Kohler or Toop equations. An extensive discussion led to the proposals that the excess free energy of an interstitial solution be defined relative to the ideal substitutional solution or relative to an interstitial positional entropy which is dependent on the structure.

Magnetic contributions – Magnetic contributions to the free energy of substitutional alloys were considered. The work of Peter Miodownik was recognized and it was proposed that he be invited to contribute at the next CALPHAD meeting in Grenoble.

Notation. A very wide range of thermochemical notations were in use by members of the group. This led to difficulties in understanding and applying specific models. It was suggested that an attempt be made to develop a universally acceptable notation in which unnecessary symbols would be avoided.

A review of the above list of topics shows that, while very significant progress has been made subsequent to CALPHAD 1, there is still much discussion on several of these original themes. In particular, it is important to realize that reliable calculations in multicomponent systems require data for the constituent binaries and ternaries which have been carefully assessed using models which are as physically realistic as possible.

A second meeting of this core CALPHAD group took place in Grenoble at the end of April, 1974. Further invited attendees were, Wolfgang Pitsch from MPI, Düsseldorf, Germany, Peter Miodownik from The University of Surrey, UK and Malcolm Rand from A.E.R.E., Harwell, UK. Etienne Bonnier and Jean-Claude Mathieu from the laboratory in Grenoble, and Oswald Kubaschewski from RWTH Aachen, also attended the meeting.

4. Importance of thermodynamic databank development

The continued developments in CALPHAD assessment of alloy (and other materials) phase diagrams was assisted by the creation of thermochemical databanks — an activity that was proceeding both side-by-side and in conjunction with CALPHAD activities [10–14]. The advent of the computer provided a perfect platform for automating the storage and retrieval as well as the assessment and application of thermodynamic data. The availability of assessed parameters for many systems also allowed easy exchange and use of data by others in the field, thereby providing a basis for calculations and continuous addition and updating of the stored parameters.

In the very early days, Kaufman had already assembled regular and subregular solution parameters, which provided reasonable assessments of many binary systems. Parameters for many superalloy systems were reported in Ref. [15], while others for a large number of transition metal systems were published in the CALPHAD journal [16], which first appeared in 1977. Hillert’s group in Stockholm had also been concerned for some time with the assessment of binary and ternary alloy systems relevant to steelmaking. Examples of early ternary assessments can be found in Refs. [17–19].

The ongoing thermodynamic databank activities at NPL and at AEA Harwell in the UK, at the University of Grenoble and IRSID, Maizières-les-Metz, in France, and at the RWTH in Aachen, Germany, had formed the basis for a French (CNRS)-funded project (1969–1974) to establish a common databank, accessible to all participants, which would provide up-to-date data for the research activities of the participating laboratories, as well as for other interested parties. The project, under the guiding hand of Etienne Bonnier, became truly European when, together with KTH Stockholm, and with significant European funding, SGTE (Scientific Group Thermodata Europe) was founded in 1979. The SGTE databank contained assessed data both for inorganic compounds and alloys and was at first accessible throughout the European Community via the EURONET telecommunications system.

The SGTE data for the elements, compiled by Dinsdale [20] now form an important basis for nearly all CALPHAD-type assessments of alloy systems carried out worldwide, while the SGTE Solution Database continues to expand with CALPHAD-type assessments for hundreds of binary, ternary and higher-order systems.

It is important to emphasize that members of SGTE were, from the beginning, also committed “CALPHADians” and that the collaboration and exchange of ideas that took place between the participating scientists at meetings of both organizations contributed significantly to the subsequent development of the computational thermochemistry software and data packages now available commercially.

Independent of the European activities, thermochemists at the Ecole Polytechnique in Montreal, Canada, were engaged in the development of their own thermodynamic databank system [14]. Their activities included CALPHAD-type assessments of a large number of oxide and salt systems, thereby including further groups of materials for which assessed thermodynamic data were becoming available.

All of the above projects contributed greatly to a dramatic increase in the acceptance and use of thermodynamic calculations in the development of new materials.

5. Software

5.1. Early phase diagram calculations

The calculation of common tangents to the Gibbs energy curves of the phases in a binary system to derive equilibrium phase boundary compositions over a range of temperatures, and hence produce a complete phase diagram, constituted a relatively straightforward mathematical problem. In the case of a ternary system, calculation of the points of contact of tangent planes to the Gibbs energy surfaces of the phases in question, corresponding to the determination of the minimum Gibbs energy of an alloy of defined overall composition, was a more time-consuming calculation process. Early Gibbs energy minimization methods for calculation of phase equilibria in higher-order alloy systems were described by Gaye and Lupis [21] and by Counsell et al. [22].

5.2. Parameter optimization software

A very great advance in the thermodynamic assessment and calculation of alloy phase diagrams was achieved when the previous hand-calculation procedure used to achieve consistency between experimentally determined thermodynamic and phase boundary values for an alloy system was superceded with the publication of *Optimization of phase diagrams by a least squares method using simultaneously different types of data,* a paper written by Lukas, Henig and Zimmermann [23]. The software described in this article was made freely available to those who wished to use it and in its original and later updated forms, the code has been responsible for assessment work on hundreds, if not thousands, of systems.

Similar parameter optimization software was written later by Jansson [24].

6. The CALPHAD journal

The first issue of CALPHAD appeared in 1977, under the editorship of Larry Kaufman. The journal has always been the primary literature source for original thermodynamic assessments of alloy systems. Articles presenting descriptions of assessments and optimized parameters for not only alloys, but also oxides, salts, aqueous systems and even organic systems still represent the major content of the journal. At the same time, the development of different solution models, the introduction of First Principles methods, and the application of thermodynamic calculations to different materials problems over the years, can be traced back to a great extent by perusal of the papers submitted to the CALPHAD Journal. A selection is presented in the following section.

7. Some developments in CALPHAD since its conception

7.1. Lattice stabilities for elements

Computer Calculation of Phase Diagrams L. Kaufman, H. Bernstein, Academic Press, New York, 1970

Lattice Stability of AX and AB_2O_4 Compounds Alexandra Navrotsky, **4** (1980) 255–264

Metastable lattice stabilities for the elements N. Saunders, A.P. Miodownik and A.T. Dinsdale, **12** (1988) 351–374

SGTE data for pure elements A.T. Dinsdale, **15** (1991) 317–425

The Ringberg workshop 1995 on unary data for elements and other end-members of solutions Bo Sundman and Fritz Aldinger, **19** (1995) 433–436

Equation of state parameters for stable and non-stable transition metal phases from universal binding energy relations J. E. Garcés and A. Fernández Guillermet, **22** (1998) 469–493

A realistic equation of state for solids. The high pressure and high temperature thermodynamic properties of MgO M.H.G. Jacobs and H.A.J. Oonk, **24** (2000) 133–147

Ab initio lattice stability in comparison with CALPHAD lattice stability Y. Wang, S. Curtarolo, C. Jiang, R. Arroyave, T. Wang, G. Ceder, L.-Q. Chen, Z.-K. Liu, **28** (2004) 79–90

Assessments of molar volume and thermal expansion for selected bcc, fcc and hcp metallic elements Xiao-Gang Lu, Malin Selleby and Bo Sundman, **29** (2005) 68–89

Ab initio lattice stabilities of some elemental complex structures M.H.F. Sluiter, **30** (2006) 357–366

7.2. Magnetism in phase diagram calculations

The calculation of magnetic contributions to phase stability A.P. Miodownik, **1** (1977) 133–158

A model for alloying in ferromagnetic metals Mats Hillert and Magnus Jarl, **2** (1978) 227–238

7.3. First principles calculations in the CALPHAD environment

A physicist's view of the energetics of transition metals D.G. Pettifor, **1** (1977) 305–324

Ab-Initio pseudopotential calculations of the structure and stability of binary alloys and intermetallic compounds J. Hafner and F. Sommer, **1** (1977) 325–340

Model predictions for the enthalpy of formation of transition metal alloys A.R. Miedema, F.R. de Boer and R. Boom, **1** (1977) 341–359

A database for enthalpies of formation of binary transition metal alloys L.H. Bennett and R.E. Watson, **5** (1981) 19–23

Comparison of pair potential and thermochemical models of the heat of formation of BCC and FCC alloys Dunbar Birnie, E.S. Machlin, Larry Kaufman and Keith Taylor, **6** (1982) 93–126

Coupled pair potential, thermochemical and phase diagram data for transition metal binary systems-VII Larry Kaufman, Bjorn Uhrenius, Dunbar Birnie and Keith Taylor, **8** (1984) 25–66

Calculation of temperature-concentration diagrams by the CV method with Lennard–Jones pair interactions C. Sigli and J.M. Sanchez, **8** (1984) 221–231

Tetrahedron treatment of the fcc lattice Ryoichi Kikuchi and Joanne L. Murray, **9** (1985) 311–348

Trends in cohesive energy of transition rare-earth metal alloys C. Colinet and A. Pasturel, **11** (1987) 335–348

Monte Carlo calculation of phase equilibria in ternary systems S.H. Lim, G.E. Murch and W.A. Oates, **14** (1990) 27–39
CVM model calculation of the Al–Mg–Ag phase diagram S.S. Lim and P.L. Rossiter, **18** (1994) 113–123
Cluster variation method in the computational materials science R. Kikuchi and K. Masuda-Jindo, **26** (2002) 33–54
Accuracy of ab initio methods in predicting the crystal structures of metals: A review of 80 binary alloys Stefano Curtarolo, Dane Morgan and Gerbrand Ceder, **29** (2005) 163–211
The Ringberg workshop 2005 on Thermodynamic Modeling and First-Principles Calculations M. Zinkevich, F. Aldinger and B. Sundman, **31** (2007) 2–3.

7.4. Developments in optimization and calculation techniques

Computational techniques for the treatment of thermodynamic data in multicomponent systems and the calculation of phase equilibria A.D. Pelton and C.W. Bale, **1** (1977) 253–273
Strategies for the calculation of phase diagrams H.L. Lukas, J. Weiss and E.-Th. Henig, **6** (1982) 229–251
Scheil reaction scheme by computer M. Hillert and B. Sundman, **14** (1990) 111–114
On a new strategy for phase diagram calculation 1. Basic principles Chen Shuang-Lin, Chou Kuo-Chih and Y.A. Chang, **17** (1993) 237–250
Calculation of constrained equilibria by Gibbs energy minimization Pertti Koukkari and Risto Pajarre, **30** (2006) 18–26.

7.5. Modelling of solutions

Influence of associate formation in alloy-melts on the thermodynamic quantities F. Sommer, **2** (1978) 319–324
Formulation of the A2/B2/D03 atomic ordering energy and a thermodynamic analysis of the Fe–Si system Byeong-joo Lee, Seh Kwang Lee and Dong Nyung Lee, **11** (1987) 253–270
A database and sublattice model for molten salts Arthur D. Pelton, **12** (1988) 127–142
Bond energy model of multiple sublattice solutions using species chemical potentials. Basic theory and relation to compound energy model W.A. Oates and H. Wenzl, **17** (1993) 35–46
Modelling of acid and basic slags Bengt Hallstedt, Mats Hillert, Malin Selleby and Bo Sundman, **18** (1994) 31–37
On putting more physics into CALPHAD solution models W.A. Oates, H. Wenzl and T. Mohri, **20** (1996) 37–45
Some properties of the compound energy model Mats Hillert **20** (1996) 333–341
The Ringberg Workshop 1996 on solution modelling Bo Sundman, Hans-Jürgen Seifert and Fritz Aldinger, **21** (1997) 139–141
Equivalence of the generalized bond-energy model, the Wagner–Schottky-type model and the compound-energy model for ordered phases F. Zhang, W. Huang and Y.A. Chang, **21** (1997) 337–348
A thermodynamic model of amorphous silicates J.A. Golczewski, H.J. Seifert and F. Aldinger, **22** (1998) 381–396
A general "geometric" thermodynamic model for multicomponent solutions Arthur D. Pelton, **25** (2001) 319–328
On the compound energy formalism applied to fcc ordering. A. Kusoffsky, N. Dupin and B. Sundman, **25** (2001) 549–565
Remarks on crystallochemical aspects in thermodynamic modeling R. Ferro and G. Cacciamani, **26** (2002) 439–458
Kinetic approach to the determination of the phase diagram of a solid solution Marija Matovic, J.C. van Miltenburg, H.A.J. Oonk and Jan H. Los **30** (2006) 209–215
Thermodynamic description and growth kinetics of stoichiometric precipitates in the phase-field approach S.Y. Hu, J. Murray, H. Weiland, Z.K. Liu and L.Q. Chen, **31** (2007) 303–312.

7.6. Software for computational thermochemistry

"ExTHERM": the interactive support package of experimental thermodynamics Josef Tomiska, **26** (2002) 143–154
Thermodynamic database MALT for Windows with GEM and CHD Harumi Yokokawa, Shigeru Yamauchi and Takafumi Matsumoto, **26** (2002) 155–166
Thermosuite Bertrand Cheynet, Pierre-Yves Chevalier and Evelyne Fischer, **26** (2002) 167–174
The PANDAT software package and its applications
S.-L. Chen, S. Daniel, F. Zhang, Y.A. Chang, X.-Y. Yan, F.-Y. Xie, R. Schmid-Fetzer and W.A. Oates, **26** (2002) 175–188
FactSage thermochemical software and databases
C.W. Bale, P. Chartrand, S.A. Degterov, G. Eriksson, K. Hack, R. Ben Mahfoud, J. Melançon, A.D. Pelton and S. Petersen, **26** (2002) 189–228
MTDATA — thermodynamic and phase equilibrium software from the National Physical Laboratory R.H. Davies, A.T. Dinsdale, J.A. Gisby, J.A.J. Robinson and S.M. Martin, **26** (2002) 229–271
Thermo-Calc & DICTRA, computational tools for materials science J.-O. Andersson, Thomas Helander, Lars Höglund, Pingfang Shi and Bo Sundman, **26** (2002) 273–312
TICP — an expert system applied to predict the formation of ternary intermetallic compounds Yao Lixiu, Qin Pei, Chen Nianyi and P. Villars, **25** (2001) 27–30
IVTANTHERMO for Windows — database on thermodynamic properties and related software Gleb V. Belov, Vladimir S. Iorish and Vladimir S. Yungman, **23** (1999) 173–180

7.7. Applications of computational thermochemistry

The effect of irradiation on the phase stability of the sigma phase L. Kaufman, J.S. Watkin, J.H. Gittus and A.P. Miodownik, 1 (1977) 281–290
Chemical thermodynamics of iodine species in the HTGR fuel particle T.B. Lindemer, **7** (1983) 87–102
Chemical equilibria for accident analysis in pressurised water nuclear reactor systems P.E. Potter and M.H. Rand, **7** (1983) 165–174
Thermodynamic calculation of atmospheric pressure and high pressure ($P = 2500$ atm) phase diagram of $LiIO_3$–$NaIO_3$ *binary system* Xiaolong Chen, Jingkui Liang, Zhan Chen, Zhiyu Qiao, Sishen Xie, Guanghui Rao and Zhongyi Shen, **15** (1991) 185–194

Table 1
Locations of past CALPHAD meetings

1973, Cambridge, USA	1974, Grenoble, France	1975, London, England	1975, Washington, DC, USA	1976, Dusseldorf, W. Germany
1977, Oxford, England	1978, Stuttgart, W. Germany	1979, Stockholm, Sweden	1980, Montreal, Canada	1981, Vienna, Austria
1982, Argonne, USA	1983, Liege, Belgium	1984, Grenoble, France	1985, Cambridge, USA	1986, London, England
1987, Irsee, W. Germany	1988, Berkeley, USA	1989, Stockholm, Sweden	1990, Amsterdam, The Netherlands	1991, Jamshedpur, India
1992, Jerusalem, Israel	1993, Barcelona, Spain	1994, Madison, USA	1995, Kyoto, Japan	1996, Erice, Sicily
1997, Palm Coast, USA	1998, Beijing, China	1999, Grenoble, France	2000, Cambridge, USA	2001, York, England
2002, Stockholm, Sweden	2003, La Malbaie, Canada	2004, Krakow, Poland	2005, Maastricht, The Netherlands	2006, Technion City, Israel
2007, The Pennsylvania State University, USA				

The SGTE Case Book — Thermodynamics at work: Edited by K. Hack, published by The Institute of Materials, **21** (1997) 449–450

The phase relations in the FeO–MgO–Al_2O_3–SiO_2 *system: assessment of thermodynamic properties and phase equilibria at pressures up to 30 GPa* O.B. Fabrichnaya, **23** (1999) 19–67

The Ringberg workshop 1997 on the application of computational thermodynamics Bo Sundman, Fritz Aldinger and Hans Jurgen Seifert, **24** (2000) 15–17

Calculation of surface tension of liquid Bi–Sn alloy using thermochemical application library ChemApp Toshihiro Tanaka, Klaus Hack and Shigeta Hara, **24** (2000) 465–474

Computational Thermodynamics and materials design Larry Kaufman, **25** (2001) 141–161

Computational thermochemistry: from its early CALPHAD days to a cost-effective role in materials development and processing P.J. Spencer, **25** (2001) 163–174

Beyond discovery: design for a new material world G.B. Olson, **25** (2001) 175–190

Application of computational thermodynamics to the analysis of waste melting processes Chunlin Chen and Masanori Tokuda, **27** (2003) 193–199

The derivation of thermo-physical properties and phase equilibria of silicate materials from lattice vibrations: Application to convection in the Earth's mantle M.H.G. Jacobs, A.P. van den Berg and B.H.W.S. de Jong, **30** (2006) 131–146.

7.8. Miscellaneous

Ortho-equilibrium and para-equilibrium phase diagrams for interstitial/substitutional iron alloys Ernst Kozeschnik and John M. Vitek, **24** (2000) 495–502

A Bayesian approach to evaluating the uncertainty of thermodynamic data and phase diagrams M. Stan and B.J. Reardon, **27** (2003) 319–323

8. Locations of past CALPHAD meetings

The growth of CALPHAD from the handful of participants at CALPHAD 1, to now include scientists from laboratories all over the world is reflected in the ever-widening geographical locations of CALPHAD meetings. These are presented in Table 1.

9. Gibbs triangle winners

CALPHAD established the Gibbs Triangle Award in 1989 in celebration of the 150th birthday of Josiah Willard Gibbs, whose year of birth was 1839.

The award, in the form of a musical triangle, was to be made every third to fifth year for outstanding contributions to studies of ternary and higher-order phase diagrams, their thermodynamic background and principles of construction as well as methods of calculation and assessment work.

The name of the award has been taken from Gibbs' composition triangle, commonly used in representing ternary phase diagrams.

The recipient is chosen by the associate editors of the CALPHAD journal together with prior recipients of the award.

Those who have received the award to date are:

Larry Kaufman (1989) Taji Nishizawa (1994) Arthur Pelton (1999)
Mats Hillert (2000) Bo Sundman (2002) Gunnar Eriksson (2007)

10. Summary

CALPHAD can justifiably claim to be one of the major success stories in the field of materials development over the last quarter century. From a previous "trial-and error" approach to designing or improving a process or alloy, the "CALPHAD method" is now widely and routinely applied as an integral part of the development process. The currently available data and software have reached a level of reliability such that, in combination with far fewer experimental measurements, thermodynamic calculations allow considerable time and costs to be saved in producing a material of the required composition and phase constitution for a particular application.

It should be emphasized that the rapid advances achieved by CALPHAD owe much to the scientific stimulation resulting from the close collaboration maintained over nearly three decades by the relatively small number of scientists participating in CALPHAD meetings and using CALPHAD calculation methods.

Those wishing to read further details of CALPHAD developments and methodology are referred to the excellent books by Saunders and Miodownik [25] and by Lukas, Fries and Sundman [26].

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