Thermochimica Acta, 214 (1993) 93–96
Elsevier Science Publishers B V , Amsterdam

The Thermo Calc Project

Bo Jansson, Björn Jönsson, Bo Sundman and John Ågren

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

ABSTRACT

The Thermo Calc project was launched more than a decade ago and is concerned with the development of software and data bases for thermodynamic calculations in non-organic systems. Calculations may be performed for a wide range of materials, for example, metals, ceramics and molten salts as well as aqueous solutions and gas mixtures. The practical use of experimental data produced by thermal analysis or calorimetry is discussed.

1. Introduction

In order to make efficient use of thermodynamic data in practical calculations it is necessary to have some method of extrapolating and interpolating the various pieces of experimantal information. A well established method for tackling this problem is the so-called Calphad technique which forms the basis for the Thermo Calc project(1) which was launched more than a decade ago.

2. The Calphad Technique

The Calphad technique involves the representation of various experimental data by means of integral Gibbs energy functions for the individual phases of a system. The actual model parameters used in the Gibbs energy expressions are obtained by an assessment procedure wherein model predictions are compared with experimental data such as phase diagram lines, heat contents, heat capacities or activity measurements. The model parameters are varied until the best fit is obtained. In Fig. 1 we show a schematic flow chart of a generalized Calphad assessment as presented by Guillermet(2). The achieved parameters are subsequently stored in a database for convenient retrival.

Phase equilibria are calculated by minimizing the total Gibbs energy of the system specified. Different thermodynamic quantities of interest are calculated by standard themodynamic methods from the various derivatives of the Gibbs energy.

3. Models

The Thermo Calc software package can handle many different models for describing the non-ideality of a phase. Examples are: the compound energy model(3), the two-sublattice ionic liquid model(4), the cell model for slags(5), the associate model(6), and the cluster variation method(7). Magnetic transitions are modelled according to Inden(8) and aqueous solutions can be treated with the Pitzer model(9).

This paper was presented at the 13th Nordic Symposium on Thermal Analysis and Calorimetry, Stockholm, Sweden, 9–11 June 1992

4.Databases

When compiling a database, it is crucial that all parameters for multicomponent systems are based on the same lower order parameters. Otherwise, data will be mutually inconsistent and useless. In Europe the Scientific Group Thermodata Europe (SGTE) is carrying out an ambitious effort to obtain a consistent and general thermodynamic database(10). In Thermo Calc one may also use a number of more specialized databases like the Fe-base for steels, the IRSID slag database or user defined databases.

5. Examples of Calculations Made with Thermo Calc

Many different kinds of calculations may be done within Thermo Calc and the results may be presented in many different ways. One may for instance tabulate a chemical reaction or just calculate a single equilibrium state. Furthermore, one may map phase diagrams or property diagrams. From the postprocessor output can be in either graphical or tabular form. Experimental data points may be superimposed upon the calculated diagrams for convenient comparision.

Fig. 2 shows an example of a calculated phase diagram together with experimental data, the circles and the stars were produced by thermal analysis. In Figs. 3 - 4 some typical calculations are compared with experimental data produced by calorimetry. Fig. 5 gives an example of yet another comparision between a calculation and experimental data.

6. Summary

A brief presentation of the software and databases developed within the Thermo Calc project was made. Furthermore, the essentials of the Calphad technique has been discussed. Finally, some examples of the use of thermodynamic data produced by thermal analysis or calorimetry has been made.

References

1. J.-O. Andersson, B. Jansson and B. Sundman: Calphad 9(1985)153
2. A.F. Guillermet: Thesis (1988), Royal Institute of Technology, 10044 Stockholm, Sweden
3. M. Hillert, B. Jansson and B. Sundman: Z. Metallkde 79(1988)81
4. M. Hillert, B. Janssson, B. Sundman and J. Ågren: Metall. Trans. 16A(1985)261
5. M.L. Kapoor and M.G. Frohberg: Arch. Eisenhüttenw. 45(1974)663
6. F. Sommer: Z. Metallkde 73(1982)72
7. B. Sundman and T. Mohri: Z. Metallkde 81(1990)251
8. G. Inden: Z. Metallkde 66(1975)725
9. K.S. Pitzer: J. Phys. Chem. 77(1973)268
10. I. Ansara and B. Sundman: The Scientific Group Thermodata Europe, Proc. Conf. CODATA, Ottawa (1986)
11. B. Jónsson and J. Ågren: Mater. Sci. Techn. 2(1986)913-916
12. A.F. Guillermet: Int. J. Thermophysics 8(1987)481-510
13. M. Wang and B. Sundman: Internal Report, Trita-Mac-484 (1992), Royal Institute of Technology, 10044 Stockholm, Sweden

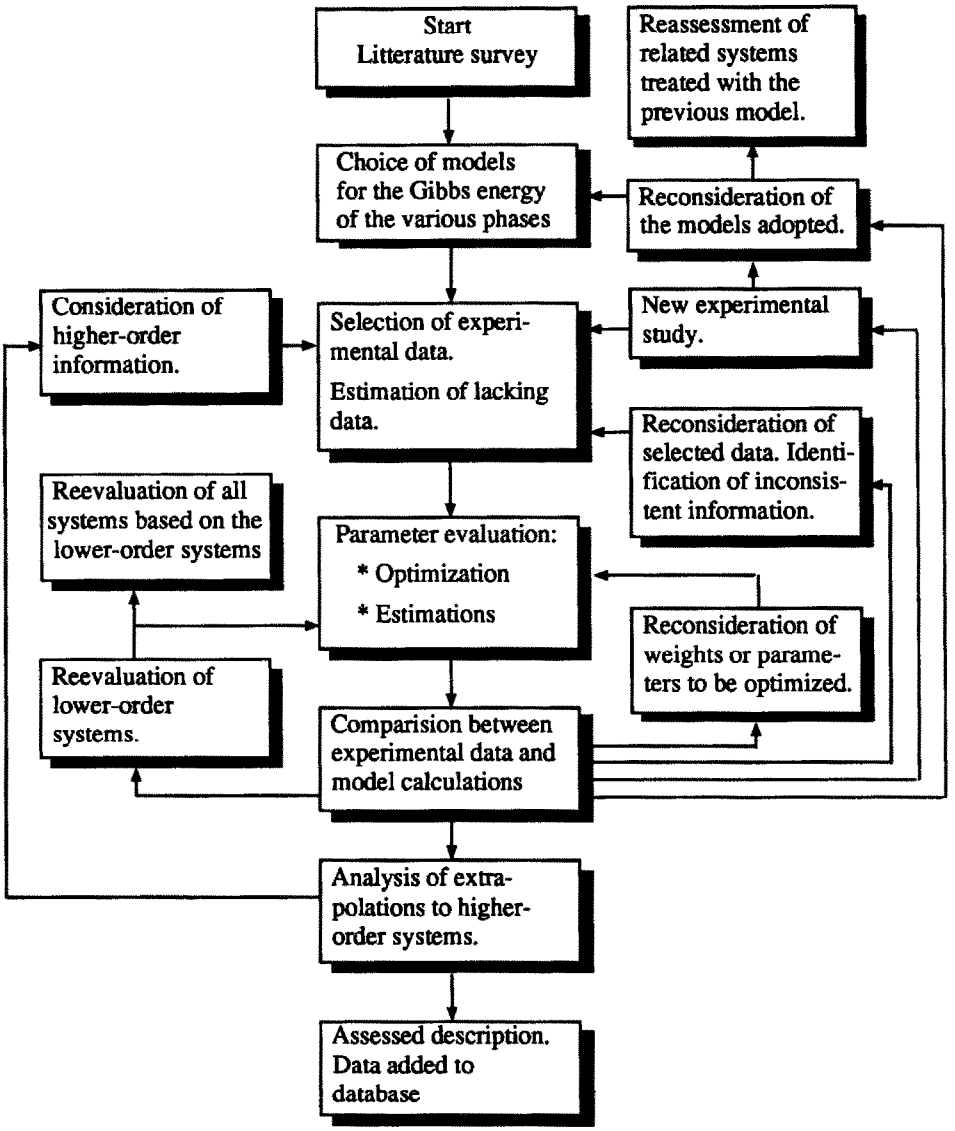

Figure 1. Flow chart over a generalized Calphad assessment.

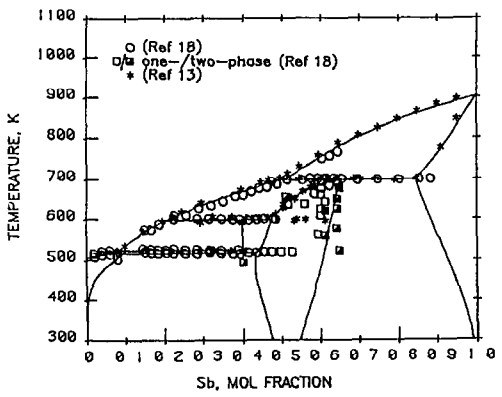

Figure 2. Comparision between calculated Sb-Sn phase diagram and experimental data, from Ref.11.

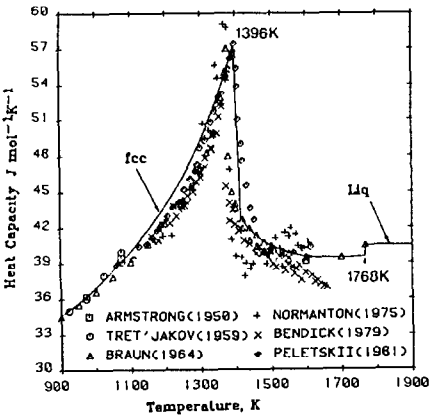

Figure 3. Comparison between calculated heat capacity of Co and experimental data. The peak in the curve is due to a magnetic transition, from Ref.12.

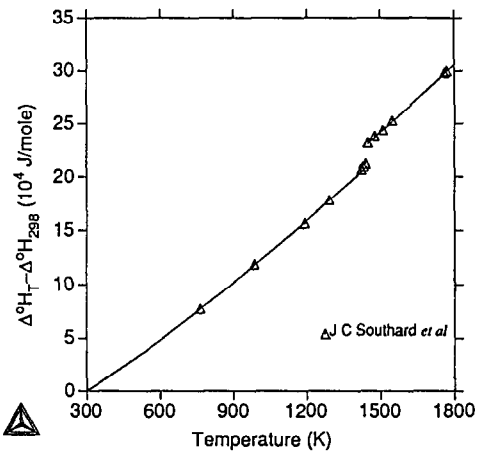

Figure 4. Comparison between calculated heat content in Mn_3O_4 and experimental data. The discontinuity in the curve is due to a first-order phase transition, from Ref.13.

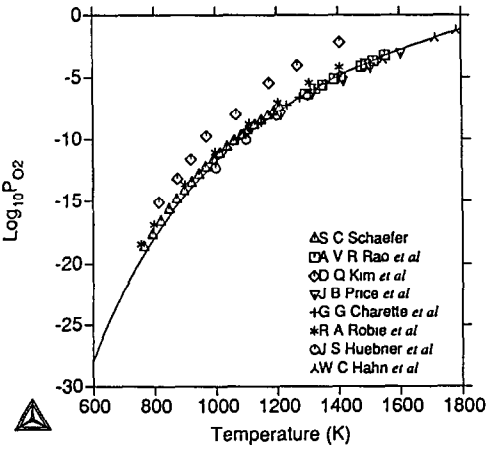

Figure 5. Comparison between calculated oxygen potential in Mn_3O_4 and experimental data, from Ref.13.