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978-0-521-86811-2 - Computational Thermodynamics: The Calphad Method

Hans Leo Lukas, Suzana G. Fries and Bo Sundman

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Computational Thermodynamics: The Calphad Method

Phase diagrams are used in materials research and engineering to understand the interrelationship of composition, microstructure, and process conditions. Computational methods such as Calphad (calculation of phase diagrams), are employed to model thermodynamic properties for each phase and simulate multicomponent multi-phase behavior in complex systems. Written by recognized experts in the field, this is the first introductory guide to the Calphad method, providing a theoretical and practical approach. Building on core thermodynamic principles, this book applies crystallography, first principles methods and experimental data to computational phase properties modeling using the Calphad method. With a chapter dedicated to creating thermodynamic databases, the reader will be confident in assessing, optimizing, and validating complex thermodynamic systems alongside database construction and management. Several case studies put the methods into a practical context, making this suitable for use on advanced materials design and engineering courses and an invaluable reference to those using thermodynamic data in their research and simulations.

HANS LEO LUKAS received his Ph.D. from the Technische Hochschule Stuttgart (now the University Stuttgart) in 1960; he continued his research there from 1964 until he retired in 1995. He has developed the BINGSS software, which is the most used optimizer for binary systems worldwide. Among numerous responsibilities over the years, he was co-editor of the journal *Calphad* from 1979 until 2003. He received the Hume-Rothery Award from the Institute of Materials, Minerals and Mining in 1993.

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Contents

	<i>Preface</i>	<i>page ix</i>
1	Introduction	1
	1.1 Computational thermodynamics	1
	1.2 The past and present, the Calphad technique	3
	1.3 The future development of databases and software applications	4
	1.4 The structure of the book	5
2	Basis	7
	2.1 Thermodynamics	7
	2.2 Crystallography	17
	2.3 Equilibrium calculations	23
	2.4 Optimization methods	42
	2.5 Final remarks	45
3	First principles and thermodynamic properties	47
	3.1 The density-functional theory (DFT) and its approximations	48
	3.2 The DFT results at 0 K	50
	3.3 Going to higher temperatures, adding the statistics	53
	3.4 Final remarks	57
4	Experimental data used for optimization	58
	4.1 Thermodynamic data	58
	4.2 Binary phase-diagram data	68
	4.3 Ternary phase-diagram data	72
	4.4 Multicomponent and other types of experimental data	75
	4.5 X-ray and neutron diffraction	76
	4.6 Mössbauer spectroscopy and perturbed angular-correlation measurements	76
	4.7 Final remarks	76
		v

vi Contents

5	Models for the Gibbs energy	79
5.1	The general form of the Gibbs-energy model	80
5.2	Phases with fixed composition	81
5.3	Variables for composition dependence	87
5.4	Modeling particular physical phenomena	91
5.5	Models for the Gibbs energy of solutions	94
5.6	Models for the excess Gibbs energy	103
5.7	Modeling using additional constituents	114
5.8	Modeling using sublattices	122
5.9	Models for liquids	146
5.10	Chemical reactions and thermodynamic models	155
5.11	Final remarks	157
6	Assessment methodology	161
6.1	Starting the assessment	161
6.2	Modeling the Gibbs energy for each phase	167
6.3	Determining adjustable parameters	192
6.4	Decisions to be made during the assessment	195
6.5	Checking results of an optimization	198
6.6	Publishing an assessed system	200
6.7	How the experts do assessment	200
7	Optimization tools	203
7.1	Common features	203
7.2	How to use BINGSS	206
7.3	The PARROT module of Thermo-Calc	219
7.4	Final remarks	240
8	Creating thermodynamic databases	243
8.1	Unary data	244
8.2	Model compatibility	244
8.3	Experimental databases	245
8.4	Naming of phases	246
8.5	From assessments to databases	249
8.6	Database management and updating	252
8.7	Existing thermodynamic databases	253
8.8	Mobility databases	253
8.9	Nano-materials	254
8.10	Examples using databases	256
9	Case studies	264
9.1	A complete assessment of the Cu–Mg system	264
9.2	Checking metastable diagrams: the Ag–Al system	274
9.3	The Re–W σ phase refit using first-principles data	276

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Frontmatter

[More information](#)

Contents

vii

9.4	A complete binary system: Ca–Mg	279
9.5	Modeling the γ – γ' phases: the Al–Ni system	285
9.6	Assessment of a ternary oxide system	287
9.7	Some notes on a ternary assessment, the Cr–Fe–Ni system	293
	<i>Appendix – websites</i>	297
	<i>References</i>	299
	<i>Index</i>	307

Preface

The idea of this book came from Professor Petzow, during the PML *Betriebsausflug* in September 1991. In a very informal way Professor Petzow invited S. G. F. (who was ready to return to Brazil after two years working with H. L. Lukas) to help H. L. L. to collect all his ideas about, and experiences with, thermodynamic optimization and put them into a book. Work on optimizations has been going on at Stuttgart for a long time, and valuable experience has been accumulated. Dr Lukas' feeling for optimizations is very well defined and one can talk about a "Lukas school for optimizations."

Later the project was enriched by the cooperation with Professor Sundman, at that time Dr. Sundman, who brought his own large experience on computational thermodynamics as well as the Stockholm group's approach to the theme with all the formalisms so well developed by Professor Mats Hillert.

The three authors were very motivated by the idea, since the lack of such a book had always made it difficult to introduce students and researchers to this field. The knowledge necessary in order to obtain a better thermodynamic description of a system is very broad, requiring a judgment of the experimental data provided by the literature and also a wise selection of the model best able to describe the experimental evidence. This judgment is difficult, but the better "educated" the assessor, the greater his ability to judge well.

The three authors have never worked together in the same institute. When B. S. visited Stuttgart during 1994, S. G. F. was already at Aachen. They have found time, however, to work together and have been meeting for many years during coffee breaks, before and after conferences, and during the Schloss Ringberg Workshops, in order to make progress with the book.

Many conferences and five Ringberg workshops were necessary to achieve the objective. During this time we were able to incorporate the most recent theoretical achievements of first-principles calculations into our procedures. When the book collecting the thermodynamic-optimization experiences of Stuttgart and Stockholm was finally sent to the Press in July 2006, S. G. F. was working in Vienna, B. S. was working in Toulouse, and H. L. L. had retired and was living in Stuttgart – and it was in time for the 80th birthday of Professor Petzow! The modeling and software has developed significantly during the writing of the book and it has been a challenge to keep it updated. Continuous updates will be provided at the website of the book.

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[More information](#)

x



The authors discussing the book in the Hexenzimmer at Schloss Ringberg in 2005, during the Thermodynamic Modeling and First-Principles Calculations Workshop organized by the Max Planck Society.

Dedication

The authors wish to dedicate this book to Ibrahim Ansara, who always managed to put a smile on the face of thermodynamics, like in the phase diagram Fig. 5.6(k).

Acknowledgments

The authors are grateful to A. Fernández Guillermet, B. Hallstedt, M. Harmelin, M. Hillert, U. Kattner, Frau O. Kubaschewski, B. Legendre, and many others for inspiration, reading parts of the book, and giving valuable comments; and to B. Böttger, N. Dupin, F. Lechermann, P. Rogl, and N. Warken for providing figures from their ongoing research work.

The figures with crystal structures have been taken from the Crystal Lattice Structures web page, <http://cst-www.nrl.navy.mil/lattice/>, provided by the Center for Computational Materials Science of the United States Naval Research Laboratory.

The triangular symbol in the left-hand corner of some diagrams indicates that the figure has been calculated by the Thermo-Calc software (Thermo-Calc Software AB, <http://www.thermocalc.com>).