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Jean-Claude Tedenac

Thermodynamics of Crystalline Materials

From Nano to Macro

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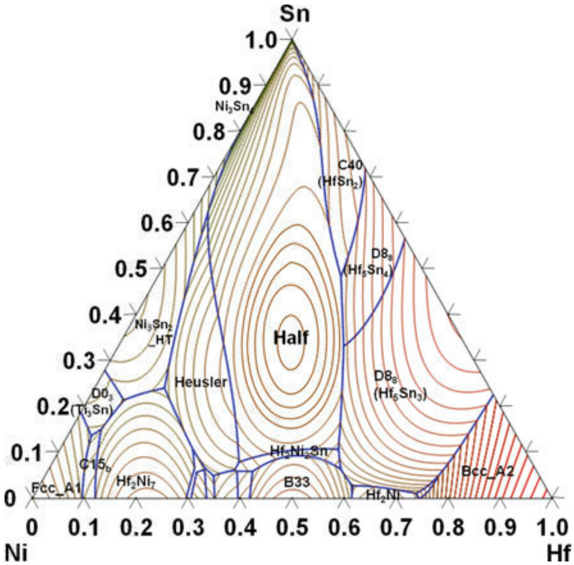

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Half
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D88
(Hf5Sn3)
D03
(Ti3Sn)
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C15b
Bcc_A2
Hf2Ni7
B33
Fcc_A1
Hf2Ni
0
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
Ni
Hf

Acknowledgments

I would like to acknowledge some colleagues and friends with whom I had in-depth scientific exchanges. All of them were influencing me, each in their own way.

Firstly, Prof. Dr. Catherine Colinet from SIMAP (INP Grenoble). For a long time, we had a lot of exchanges and discussions concerning the field of Thermodynamics of Materials and Ab initio calculations.

Secondly, Dr. Pascal Yot (University of Montpellier) was a former student in my courses. He checked precisely the crystallography chapter and corrected the draft of all chapters of the document.

I would not want to forget my friends who passed away prematurely, Dr. Ibrahim Ansara from Grenoble (Fr) and Dr. Gunter Effenberg from MSIT Stuttgart (Ge). They were very well versed in phase diagram studies, and we enjoyed all discussions we had, especially in the «Tagungsstätte Schloss Ringberg (Germany)».

Basically, this book is based on the courses I've made during ten years at the University of Montpellier at the levels of Master and Doctorate, during which I was able to observe and analyze the student's reactions to this part of science.

Thermodynamics of materials is a particular science. It always joins strongly physics to chemistry. The proven bestsellers, Alan Prince (Alloy Phase Equilibria) and Mats Hillert (Phase Equilibria, Phase Diagrams and Phase Transformations: Their Thermodynamic Basis), are consistently praised as the most clearly written books available for improving the knowledge of materials.

Some other references to excellent books will be cited as well in the text.

General Introduction

Basis and New Trends in Thermodynamics and Phase Diagrams

The purpose of this book concerns the presentation of modern aspects of the study of phase diagrams and equilibria. Currently, the description of phase equilibria in the twenty-first century requires a multidisciplinary approach linking crystallography and thermodynamics and integrating quantum mechanics.

The history of one of the most exciting sciences of material classes can be traced back to the nineteenth century when J. Willard Gibbs (October 1875–May 1876) (1) discovered the basis of «Equilibrium of Heterogeneous Substances» and published it in the journal: Transactions of the Connecticut Academy of Arts and Sciences. This remarkable first paper developed the theory of chemical thermodynamics and provided the basic theory for the development of this part of physical chemistry.

In the field of metallurgy, the Gibbs theory application provided the basement of the knowledge in multicomponent alloy phase equilibria, and this feature entails the evolution of phase diagrams and applications during the twentieth century. In the twenty-first century, with the progress of experimental determinations and the rise of advanced calculation methodology, the application of the CALPHAD method is presently generalized in alloys and ceramics while in polymer systems the work is not well established. The properties of phase relationships were predicted by simple analysis of the thermal properties of mixtures with good accuracy. More recently, those properties were investigated with modern tools such as physical measurements (electron microscopies, Castaing microprobe and X-Ray diffraction) and quantum mechanics.

The plotting of phase diagrams of two- and three-component systems is not so easy. In both coordinate systems (composition/temperature and/or other coordinates, which are thermodynamic parameters of the phases), the total pressure in the system, molar volume, chemical potentials of components, etc. This is the more pertinent approach to consider and classify.

This book does not claim a replacement for already published books (of quality!). Its objective is to make an analysis of this part of science at a level such that students or even researchers have some difficulties in approaching certain phenomena and experiences in phase equilibria. It is divided into five chapters. Two of them state what is necessary to know in crystallography and thermodynamics in order to apply them to the matter of phase diagrams. Two other chapters are more constructed as guides to the application of the CALPHAD method. They are a gateway to more technical works. Finally, I will present, in a fifth chapter, a small contribution to quantum calculations. But in such a case and to go further, it will be really necessary to use more specialized books.