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Phase Diagrams Could Not Be Found

Crystal Structure Tables for Systems Where Phase Diagrams Could Not Be Found
As Publisher of the first edition of *Desk Handbook: Phase Diagrams for Binary Alloys*, I am honored that Dr. Okamoto asked me to make a few comments for this second edition. “Hiro,” as I know him, has been involved with ASM publications for more than 30 years, and for a period of about five years, in the late 1980s and early 1990s, he was employed by ASM as our “expert” in binary phase diagrams. He had the idea of publishing a handbook, updated, and only including diagrams and some crystallographic data. His interest was in providing a single volume, having all diagrams in atomic percent for the primary axis, and offering a quick look-up with key references for those who wanted to “dig deeper” into the literature. I am pleased that ASM is publishing a second edition of the original volume, with additional updates.

I am aware of no other living person who has evaluated, examined, and edited more diagrams than Hiro Okamoto. That alone qualifies him to be the editor of this volume. However, his scientific background, combined with his job of looking at every single known binary diagram, caused him to see some patterns occurring in the literature. There were many situations where diagrams were drawn incorrectly, based on thermodynamic arguments. As a result he decided to write, in collaboration with Professor Thaddeus Massalski* of Carnegie Mellon University, what I consider to be a classic paper in the *Journal of Phase Equilibria* in 1991, regarding thermodynamically improbable diagrams (see list below for reference).

Following this publication, Dr. Okamoto and Professor Massalski continued to write instructive articles for the phase diagram community. Specifically, the following articles are of importance:


If you have not read these papers, and you are using phase diagrams, you should consult them because they are extremely instructive. In particular, the last paper on systems requiring further study, is very revealing, pointing out issues and contradictions in published diagrams and the need for further work in many, many systems.

Based on this background, his unique situation in having viewed every diagram, seen the problems in existing diagrams, and his passion for improving the published binary diagrams, you can see why it was important for a second, updated edition of the Desk Handbook to be published, I think you will find it will meet the original objectives stated by Dr. Okamoto, and it provides another important and continuing publication for ASM, as they continue to provide periodical publications and reference material for the phase equilibria community.

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* Professor T.B. Massalski was the Editor-in-Chief of the Data Program for Binary Phase Diagrams for about 15 years, a joint program between ASM and NIST (U.S. National Institute of Standards and Technology), involving about $10 million in expenditures towards evaluating and publishing binary phase diagram information. He is one of the most knowledgeable persons in phase equilibria in the world. As you will know from having read the other introductory materials, he is also the Editor-in-Chief of *Binary Alloy Phase Diagrams*, the most important compilation of binary phase diagrams, text, and data in recent times.
About the Editor

Dr. Hiroaki Okamoto is co-editor of ASM’s primary binary phase diagrams reference work, the three-volume set *Binary Alloys Phase Diagrams*, Second Edition [Massalski2], and the electronic edition of this work, *Binary Alloy Phase Diagrams, Second Edition, Plus Updates*, on CD-ROM. He has personally evaluated and published phase diagrams and related data for more systems than any other living professional, completing 505 evaluations.

Dr. Okamoto has also published classic articles on common mistakes made in drawing phase diagrams, including “Thermodynamically Improbable Phase Diagrams,” “Reevaluation of Thermodynamic Models for Phase Diagram Evaluation,” and “Guidelines for Binary Phase Diagram Assessment” (*Journal of Phase Equilibria, 12*(2), 12*(6), and 14*(3), respectively). He has been Supplemental Literature Review Editor for *Journal of Phase Equilibria and Diffusion* since 1991.

Presently professor, Department of Information Management, Asahi University, Mizuho-shi, Gifu, Japan, Dr. Okamoto was senior technical editor, Alloy Phase Diagram Program, ASM International, from 1987 through 1993. He obtained his master’s degree in applied physics from Nagoya University in 1965, and his doctorate in metallurgy from the University of Illinois in 1971. Earlier in his career, he worked on the evaluation of binary gold systems at Carnegie-Mellon University in Pittsburgh and on the evaluation of beryllium alloy systems at the Lawrence Berkeley Laboratory in California. He was editor of *Phase Diagrams of Binary Iron Alloys* (ASM International, 1993), and co-editor of *Phase Diagrams of Binary Gold Alloys, Phase Diagrams of Binary Beryllium Alloys*, and *Phase Diagrams of Binary Indium Alloys and Their Engineering Applications* (ASM International, 1987, 1987, and 1991, respectively). He was also a co-editor of the 10-volume *Handbook of Ternary Alloy Phase Diagrams* (ASM International, 1995).
Preface

Binary alloy phase diagrams have been studied for more than 100 years since ca. 1900. The wealth of knowledge accumulated experimentally and theoretically in this period was assessed and summarized in various compendia. *Binary Alloy Phase Diagrams, Second Edition*, edited by T.B. Massalski, H. Okamoto, P.R. Subramanian, and L. Kacprzak, and published by ASM International in 1990, hereinafter referred to as [Massalski2], was regarded as one of the most extensive collection of binary alloy phase diagrams and has been used as a convenient and dependable tool in academics and industry for research, development, design, and other purposes for various materials in wide areas related to material sciences.

Because [Massalski2] in a three-volume set was heavy and rather difficult to handle for quick references, this author published *Desk Handbook: Phase Diagrams for Binary Alloys* in 2000, in which the size of the phase diagrams was reduced to 60 percent of that in [Massalski2] in order to accommodate three phase diagrams on each page. New or updated phase diagrams collected in the period from 1990 to 2000 were also included. For each phase diagram, crystal structures of phases existing in the system were listed and only one data source was usually given. In this way, key information on binary alloy phase diagrams could be conveniently assembled in one volume.

Ten years have passed since the Desk Handbook described above was published. In the meantime, the author introduced new and updated binary alloy phase diagrams in Section III of the *Journal of Phase Equilibria and Diffusion* at a rate of approximately 50 diagrams per year. In addition, many pieces of information leading to partial modification of phase diagrams became available. Therefore, it has become almost impossible to access the most up-to-date information on binary alloy phase diagrams through the first edition of the Desk Handbook and many volumes of the *Journal of Phase Equilibria and Diffusion*. Accordingly, this author proposed publishing this second edition of the Handbook. In summary, this second edition includes phase diagrams for 2,421 systems, in which about 450 phase diagrams have been updated. Among these, 87 phase diagrams were unknown when the first edition was published.

The format and policy for presenting the phase diagram, crystal structure data, and key reference are the same as in the first edition. The phase diagram is presented in terms of atomic percent. The weight percent scale is shown with a secondary-axis. Among various modifications of phase diagrams available for one particular system, the “best” phase diagram was selected by this author based on the current standard. An even better diagram will certainly become available in the future because almost all phase diagrams have more or less unlikely features according to the criteria summarized by this author (see below). Also, it must be noted that the updated phase diagram has not been critically evaluated. It is recommended that the reader view the new phase diagram with caution. It may look more normal from the thermodynamic point of view, but it is often the case that the phase boundaries are not supported experimentally. The reference article and other articles quoted there should be helpful in judging the reliability of the updated phase diagram. Crystal structure data for updated phase diagrams were taken from the same source as for the phase diagram whenever available. *Pearson’s Crystal Data — Crystal Structure Database for Inorganic Compounds*, edited by P. Villars and K. Cenzual (ASM International), was used as an auxiliary source. The reference was chosen so that all information on a particular system becomes available from the minimum number of sources (typically one). Two or more sources are given when all information cannot be reached by tracking back from either one of the sources. Two sources are also given when the phase diagram data and crystal structure data cannot be reasonably compromised (for example, Ge-K system).
In conjunction with Professor Massalski of Carnegie-Mellon University, this author published four articles for finding unlikely features in phase diagrams:


Many problems pointed out in these articles have been eliminated in the diagrams updated in this edition. However, many such unlikely features still remain. In order to help the reader find them quickly, “Impossible and Improbable Forms of Binary Phase Diagrams” are shown in the front section of this Handbook with minor modification from that in the first edition. Key points in the above-mentioned four articles are summarized here. Also, “Introduction to Alloy Phase Diagrams” by the late Hugh Baker of ASM is reprinted in the front section as a convenient reference to the knowledge of phase diagrams and crystal structures.

As in the first edition, in the last part of this handbook crystal structures are shown for the systems for which the phase diagram data are not available. Additional research on phase diagrams is expected for these systems.

Great care was taken to eliminate errors in phase diagrams and crystal structure data with the elaborative assistance of Japanese Alloy Phase Diagram Committee members Professor Seiji Miura of Hokkaido University and Professor Hiroshi Ohtani of Kyushu Institute of Technology. Nevertheless, it is very likely that there are still typing errors and drawing errors in this handbook. Information on such errors will be very helpful for possible future revision. Please send any such information via e-mail to Books@asminternational.org.

Lastly, the author would like to express thanks to Mary Anne Fleming, Madrid Tramble, and Scott Henry of ASM International, Materials Park, Ohio, USA; Professor T.B. Massalski of Carnegie-Mellon University, Pittsburgh, Pennsylvania, USA; and K. Ishida of Tohoku University, Sendai, Japan, for their unchanging cooperation and assistance in materializing this publication. The Miyata Research Grant from Asahi University, Gifu, Japan, facilitated the publication of this Handbook. This author greatly appreciates the generous contribution.

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