Crystallographic and Phase Equilibria Databases

Crystallographic data models are used on a daily basis to visualize, explain and predict the behavior of chemicals and materials, as well as to establish the identity of unknown phases in crystalline materials. Phase diagrams are used throughout the ceramics industry to understand and control the complex phenomena which increasingly underlie advanced industrial material production and materials performance. Literally tens of thousands of structures and phase diagrams have been reported in the literature, all with varying degrees of reliability and completeness. This project develops, maintains, and disseminates comprehensive, critically-evaluated data in printed and in modern computerized formats, along with scientific software to exploit the content of these databases.

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The NIST Structural Database (NSD) and Inorganic Crystal Structure Database (ICSD) are comprehensive collections of crystal structures covering the literature from 1915. The ICSD database system now includes chemical and 3-dimensional structure information for more than 85,000 inorganic materials. The NSD database updates this year doubled the accessible data to more than 16,000 entries. These data and scientific software are licensed to instrument manufacturers, software vendors, and other third-party distributors as well as to individual researchers in industry and academia.

To meet the need for reliable phase diagram data, the NIST Phase Equilibria Data Center and the American Ceramic Society (ACerS) jointly publish a series of critically evaluated collections of phase diagrams. The series "Phase Equilibria Diagrams," originally published under the title "Phase Diagrams for Ceramists" (1964-1992), provides current, evaluated data on the phase equilibria of ceramics and related materials. The publications also provide bibliographic data, graphical representations, and analytical capabilities so that researchers have access to reliable, up-to-date data for use in designing, applying, analyzing, and selecting those materials. The published portion of the database includes more than 15,000 entries with over 20,000 phase diagrams contained in twenty-one books and a CD-ROM – over 53,000 units have been sold world-wide. Approximately 1000 new entries are collected from the primary literature each year.

Database products completed this year include *Volume XIV: Oxides*, edited by Robert S. Roth and Terrell A. Vanderah. This volume contains more than 1200 evaluated diagrams and more than 800 descriptive commentaries on oxide systems, primarily from literature published from the early 1980's through 2004. Volume XIV complements the earlier blue books on oxide systems (I-IV, VI, XI, XII, XIII), Annuals 91-93, and the topical publications on High T_c Superconductors, Zirconium and Zirconia Systems, and Electronic Ceramics I. Systems in this volume include a wide variety of metal, non-metal, and semi-metal oxides as well as numerous aluminates, silicates, and ferrites.

Also expected in 2005 is the release of version 3.1 of the CD-ROM Database (NIST Standard Reference Database Number 31), which will provide customers with comprehensive coverage of all diagrams and commentaries published to date, including Volume XIV.

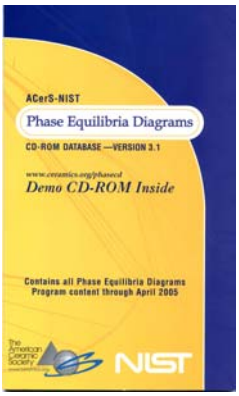

Figure 1: *Demonstration disk for Phase Equilibria Diagrams CD-ROM Database Version 3.1 (NIST Standard Reference Database Number 31), released in May 2005. This promotional item provides customers with a complete and searchable cumulative index for all published material. In addition, a small portion of the database (Annual 92) is included for customers to sample using the full functionality of the application.*

Future database products include CD-ROM versions of selected books (High T_c Superconductors, Zirconium and Zirconia Systems, and Electronic Ceramics I), and a topical slice through the database, Phase Diagrams for Fuel Cells.

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