

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 modern computerized formats, along with scientific software to exploit the content of these databases.

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The Inorganic Crystal Structure Database (ICSD) is a comprehensive collection of crystal structures covering the literature from 1915. The ICSD database system now includes chemical and 3-dimensional structure information for more than 65 000 inorganic materials. The 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. Additional information about the ICSD can be found in the Technical Highlights section of this report.

To service 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. These 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 materials. The published portion of the database includes about 16 000 entries with 26 000 phase diagrams contained in nineteen 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.

Currently underway is a complete modernization to replace the outdated 1980's system with an integrated production facility using a relational structure that will facilitate electronic publishing in a variety of formats, including a web-based version. Much of this year's effort has involved assisting and working with on-site ACerS staff to design and build the new system, which must incorporate all of the scientific data relationships embodied in the original database.

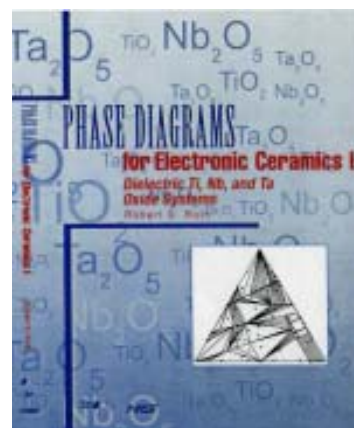


Figure 1: The latest volume in the series "Phase Equilibria Diagrams" features systems of major interest to the fields of dielectric, ferroelectric, and piezoelectric ceramics.

The latest database products completed this year include the topical volume, *Phase Diagrams for Electronic Ceramics I: Dielectric Ti, Nb, and Ta Oxide Systems*, edited by R.S. Roth (see Figure 1). This is the first volume of a new collection of phase diagrams focused on the increasingly important field of electronic ceramics. More than 1100 diagrams are presented along with commentaries written by knowledgeable associate editors. Also completed this year was an updated *Cumulative Index 2003* which provides comprehensive indexing of published equilibria data sorted by chemical system and author. In preparation is "Volume XIV — Oxides" (2004) which will contain a wide variety of metal, non-metal, and semi-metal oxide systems — more than 900 entries with 1300 diagrams are already available for inclusion.

Contributors and Collaborators

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