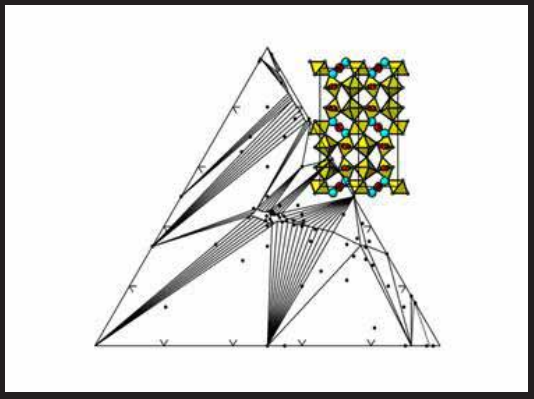
Ceramic Phase Equilibrium Data

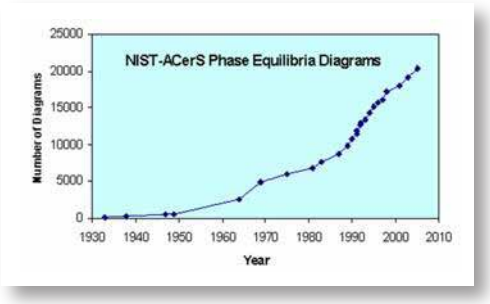
Objective

Our objective is to compile, evaluate, determine, and disseminate phase equilibrium data to facilitate and optimize the development, processing, and usage of advanced ceramic materials. By delineating the conditions (chemical composition, temperature, pressure, and atmosphere) under which pure compounds and their mixtures occur, phase equilibrium data provide essential thermochemical guidance for the technical exploitation of ceramic materials.



Impact and Customers

- Advanced ceramics are critical enabling materials for a wide spectrum of devices and systems for electronic, communications, energy, medical, and chemical purification applications.
- According to one industrial customer, "…the availability of the diagrams, particularly in the CD-ROM format, has resulted in decreased development costs, decreased time to market, decreased manufacturing costs, improved quality, and increased product functionality for our customers."
- Since 1933, NIST scientists have collaborated with the American Ceramic Society (ACerS) to meet the need for reliable phase diagram data by jointly publishing a series of critically evaluated collections of phase equilibrium diagrams.



NIST National Institute of Standards and Technology

The American Ceramic Society

Approach

Phase equilibrium data are used throughout the ceramics industry to understand and control the complex phenomena that underlie the production and performance of advanced materials. Phase diagrams serve as maps of the equilibrium chemical and structural behaviors exhibited by materials and provide critical starting information for the rational design of materials processing schemes, quality assurance efforts, and optimization of the physical and chemical properties of advanced materials. The Phase Equilibria Diagrams series (NIST Standard Reference Database 31) provides critical written commentaries, evaluated graphical representations, bibliographic data, and analytical capabilities. The published portion of the database now includes over 21,000 phase diagrams contained in 21 books and a CD-ROM. Activities in the Ceramics Division Data Center include continuous addition of new database content (about 1000 new entries per year), dissemination of the data in printed and digital formats, and development of scientific software to facilitate access to and use of the data.

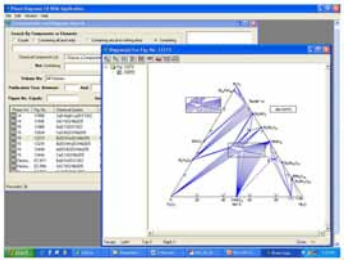
CERAMICS

Accomplishments

Recent activities in the Data Center have concentrated on using a newly redesigned Content Management System (CMS) to produce an updated version of the CD-ROM database.

Version 3.2, Phase Equilibrium Diagrams Database (SRD 31)

The new version of the database was released in December 2008 and contains 817 new figures with approximately 1,200 new diagrams, bringing the total number of diagrams in the database to more than 21,000. The new diagrams include oxide as well as non-oxide systems such as chalcogenides and pnictides, phosphates, salt systems, and mixed systems of these various ceramic materials classes.



SRD 31 provides evaluated graphical representations of phase equilibrium data in addition to written commentaries.

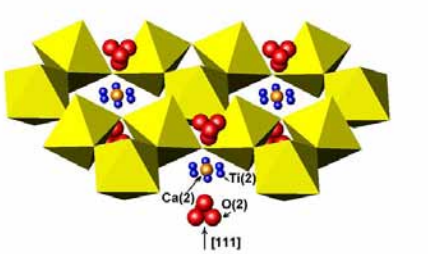
The searchable CD includes all the information previously printed in the 21 hard-copy volumes of the series, as well as additional features such as export capability. Beginning with this release, books will no longer be produced, and all new content will be published electronically. However, since the books featured the highest quality graphics, the CD-ROM now provides a .pdf version for all newly published and revised figures.

Version 3.2 of SRD 31 provides the customer with a .pdf version of the figure with blue-book highest-quality graphics.

The .pdf files are identical in format to the previously published books with full commentary text, references, and plotter-quality diagrams.

With the phase-out of hard-copy products, the Data Center is now poised to continuously release new content for advanced materials in a range of classes including oxides, chalcogenides, nitrides, borides, carbides, phosphides, and salts, as well as for mixed systems including two or more of these classes. Publication will now take place as periodic updates of the comprehensive CD-ROM developed on-site at NIST, and on-demand uploads to a web version of the database developed off-site by the American Ceramic Society.

Recent experimental phase equilibrium research has included studies of dielectric ceramic systems of interest to components for communications systems. Studies of the CaO:TiO_2:Nb_2O_5 system confirmed the formation of six ternary phases: pyrochlore ($A_2B_2O_6O'$), and five members of the (110) perovskite-slab series $Ca_n(Ti,Nb)_nO_{3n+2}$, with n = 4.5, 5, 6, 7, and 8. Relations in the quasibinary $Ca_2Nb_2O_7$-$CaTiO_3$ system were determined in detail. The practically important ceramic $CaTiO_3$ forms solid solutions with $Ca_2Nb_2O_7$ as well as $CaNb_2O_6$, resulting in a triangular single-phase perovskite region. Structural refinement of the pyrochlore $Ca_{1.46}Ti_{1.38}Nb_{1.11}O_7$ using single-crystal X-ray diffraction data were carried out, and indicated that Ti mixes on the A-type Ca sites as well as on the smaller octahedral B-type sites. Ca occupies the ideal 16d position, but Ti is displaced 0.7 Å to partially occupy a ring of six 96g sites, thereby reducing its coordination number from eight to five. The O′ oxygens in both pyrochlores were displaced 0.48 Å from the ideal 8b position to a tetrahedral cluster of 32e sites.



Local structure (displacive disorder) in the Ca-Ti-(Nb,Ta)-O pyrochlore; possible sites for displaced atoms denoted by rings of blue (Ti) and clusters of red (O) spheres

The Ca-Ti-(Nb,Ta)-O pyrochlores exhibited dielectric relaxation similar to that observed for a number of Bi-containing pyrochlores, which also exhibit displacively disordered crystal structures. Observation of dielectric relaxation in the Ca-Ti-(Nb,Ta)-O pyrochlores suggests that it arises from the displacive disorder, as opposed to the presence of polarizable lone-pair cations such as Bi^{3+}, as has been commonly assumed.

Learn More

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Publications

ACerS-NIST Phase Equilibria Diagrams CD-ROM Database *Standard Reference Database 31* Version 3.2, December 2008, www.nist.gov/srd/nist31.htm, www.ceramics.org/phase. A free demonstration CD is available upon request.

Roth RS, Vanderah TA, Bordet P, Grey IE, Mumme WG, Cai L and Nino JC *Pyrochlore Formation, Phase Relations, and Properties in the CaO-TiO_2-$(Nb,Ta)_2O_5$ Systems* J. Solid State Chem., 181: 406 (2008)

Vanderah TA, Guzman J, Nino JC and Roth RS *Stability Phase-Fields and Pyrochlore Formation in Sections of the Bi_2O_3-Al_2O_3-Fe_2O_3-Nb_2O_5 System* J. Am. Ceram. Soc., 91: 3659 (2008)

Burton BP and Nishimatsu T *First-Principles Phase Diagram Calculations for the System $NaNbO_3$-$KNbO_3$: Can Spinodal Decomposition Generate Relaxor Ferroelectricity?* Appl. Phys. Lett., 91: 092907 (2007)