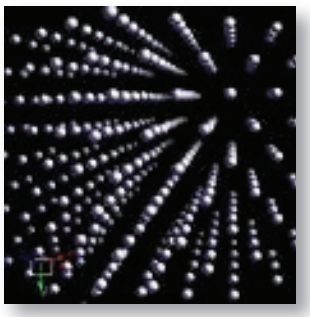
Crystallographic Databases

Objective

Our objective is to provide critically evaluated, comprehensive crystal structure databases to enable materials identification required for the development of inorganic materials and devices. Our goal is to design, populate, and disseminate these NIST standard reference databases in forms that can be readily incorporated into commercial X-ray, neutron, and electron diffraction instruments.

Impact and Customers

- Components and devices used in a broad spectrum of technology sectors such as health care, communications, energy, and electronics are manufactured from crystalline inorganic materials. The development of advanced materials with new or improved properties for such components and devices requires accurate crystal structure data.



- NIST collaborates with Fachinformationszentrum Karlsruhe (FIZ), Germany, on the collection, formatting, evaluation, and distribution of crystal structure data in the form of the Inorganic Crystal Structure Database (ICSD), Standard Reference database (SRD) 84.

- Leading vendors of X-ray and electron diffraction measurement instrumentation and software distribute NIST crystal structure databases with measurement instruments or programs, typically as analysis options.

Approach

NIST develops and provides crystal structure information in the form of three standard reference databases (SRD's): SRD 3 (NIST Crystal Data), SRD 83 (NIST Metals Structural Database), and SRD 84 (FIZ-NIST Inorganic Crystal Structure Database). SRD 3, although limited to crystallographic unit cell parameters and phase composition, is the most comprehensive in terms of materials classes, covering inorganic and organic materials, with about 250,000 entries. SRD 83 contains full crystallographic and atomic position information for about 60,000 metallic and intermetallic materials. SRD 84 contains full crystallographic and atomic position information for about 100,000 inorganic non-metallic materials. NIST continually develops scientific algorithms to evaluate crystal structure data, updates the three databases, and makes the databases available in a variety of formats.

NIST

FIZ KARLSRUHE

CERAMICS

Accomplishments

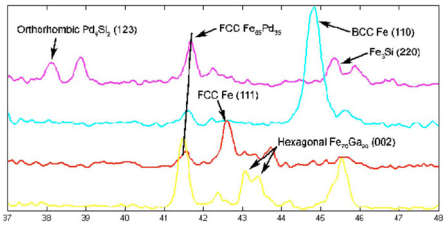
Development of advanced inorganic materials necessarily begins with the preparation and identification of constituent phases. Crystalline phases can be identified by their characteristic diffraction patterns by comparison with crystal structure data already determined for known phases. An estimated 20,000 X-ray diffractometers and a comparable number of electron microscopes are used daily to generate large amounts of experimental data that are compared with information derived from crystal structure databases to accurately identify phases.

Since 1997, Fachinformationszentrum Karlsruhe (FIZ) and NIST have collaborated in the collection, critical evaluation, consistent formatting, and distribution of 2,000 to 10,000 new and revised inorganic non-metallic crystal structures per year, released twice-yearly as updates to SRD 84, FIZ/NIST Inorganic Crystal Structure Database, ICSD.

In May 2008, FIZ and NIST entered into a new agreement for collaboration in the production and distribution of SRD 84, ICSD. This agreement was critical as it formalized NIST's added role in providing metals data to FIZ for incorporation into ICSD, thereby generating a single, interoperable, inorganic crystallographic database including both metallic and non-metallic phases.

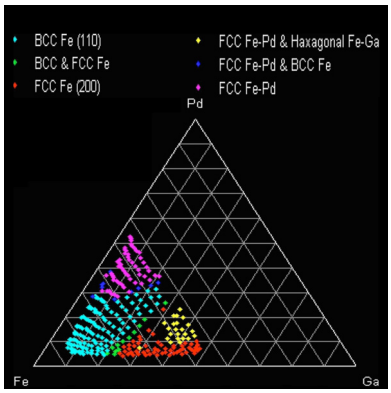
This year, about 6,000 metals entries from NIST SRD 83 (NIST Metals Structural Database, "Metals") were evaluated, standardized and delivered to FIZ, initiating this collaborative effort to incorporate these entries into SRD 84, ICSD. For the 6,000 entries, 1,249 entries with non-integral Z were resolved, 1,742 entries had multiple site-occupancy-factor issues, and 167 space group symbols were transformed to ICSD space group symbols. Metals data were mapped onto the ICSD scientific and database design; Metals Remarks were hand-edited into ICSD Standard Remarks as well as the ICSD Comments.

The combinatorial approach has been used to discover new materials phases and to perform rapid mapping of composition-structure-property relationships in complex materials systems. Collaborative work with the University of Maryland focused on interfacing and integrating combinatorial experimental data with the crystallographic databases available at NIST. As an example system, we looked at a region of the Fe–Ga–Pd ternary system. Statistical analysis tools were used to perform cluster analyses on experimental X-ray diffraction patterns collected from thin-film composition spreads. We used the composition to select crystallographic information from the SRD 83, SRD 84 databases. These data were used to calculate the theoretical diffraction data which, in combination with the results of the statistical analyses, enabled the identification of phases in the entire composition range. In this way, large fractions of compositional phase diagrams for the ternary metallic alloy system could be mapped from X-ray diffraction data collected from the combinatorial materials library.



Representative patterns after clustering in the FeGaPd system

Thus, the arduous analysis and classification of hundreds of patterns is reduced to a much shorter analysis of only a few patterns. The ultimate goal of our efforts is to reach a point where the analysis of hundreds of patterns automatically identifies all of the pure phases present in a system and quantifies each phase.



Mapping of FeGaPd phases on the compositional spread diagram

Learn More

Xiang Li
Alan Mighell

Vicky Lynn Karen
(Ceramics Division)
(301) 975- 6255
vicky.karen@nist.gov
www.nist.gov/ceramics

Publications

NIST Standard Reference Database 84 - FIZ/NIST Inorganic Crystal Structure Database; Release 2008/1 (103,679 entries); NIST contributors: Karen VL, Li X and Belsky A; http://www.nist.gov/srd

Long CJ, Hattrick-Simpers J, Murakami M, Srivastava RC, Takeuchi I, Karen VL and Li X *Rapid Structural Mapping of Ternary Metallic Alloy Systems Using the Combinatorial Approach and Cluster Analysis* Rev. Sci. Instrum., 78 072217 (2007)

Desiraju GR, Chair, Committee for Crystallographic Databases, International Union of Crystallography (Members: Allen F, Berman H, Duax B, Faber J, Karen VL, Kostorz G, McMahon B, Rodgers J and Villars P) *Report of the Executive Committee for 2006* Acta Cryst., A63 484-508 (2007)

Jeffrey GA and Karen VL *Crystallography* Chapter 9 from AIP Physics Desk Reference, Edited by Cohen ER, Lide DR and Trigg GL, 3rd Edition, 306-348 Springer (2003)