

NIST Releases Crystallography Database for Over 60,000 Metals and Intermetallics

Crystallographic databases provide researchers and instrument manufacturers with critically evaluated lattice parameter and atomic positional data that describe the three dimensional arrangement of atoms that constitute a crystal. Structural data may be used for materials modeling, as input for simulated diffraction patterns, and diagnostically for material or phase identification. Through more than five years of meticulous evaluation studies, the NIST Ceramics Division (852) has helped to ensure that researchers and instrument manufacturers will have the most comprehensive and highest quality data available.

The NIST Structural Database (NSD) is a comprehensive collection of crystal structures for metals and intermetallics. This year, NIST reached a long-awaited goal and released data on an additional 40,000 materials, bringing the total number of materials in the database to over 60,000. These NSD data were delivered to instrument manufacturers and software vendors for dissemination to the research community. The entire data set was evaluated with respect to measurement uncertainty, symmetry conventions, and data consistency. Upgrades to the data set include improved standardization of the data provided for each structure and additional data fields for each entry. Re-design of the database was undertaken with specific attention to the needs of instrument manufacturers who utilize the NSD as an analytical component of X-ray and electron diffraction instruments.

In collaboration with FIZ-Karlsruhe, Germany, NIST also produces the FIZ/NIST Inorganic Crystal Structure Database (ICSD), a comprehensive collection of data for inorganic crystalline materials. Although the original definition of the ICSD specifically excluded metals and intermetallic crystalline materials, with NIST's December 2006 delivery of the NSD to collaborators in FIZ-Karlsruhe, the definition of the FIZ/NIST ICSD has been changed to cover all categories of non-organic materials including inorganics, metals, intermetallics and minerals. Further enhancements of the NSD through continued data evaluation, transformation, and standardization, and database design are planned as the NSD is subsumed into the FIZ/NIST ICSD over the coming years. This accomplishment marks the beginning of a long-term plan to create and disseminate one comprehensive crystallographic database for all non-organic materials to benefit researchers worldwide.

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