

# CONFIDENCE COMES WITH GREAT RESULTS



**Before PDF-4+**



**After PDF-4+**

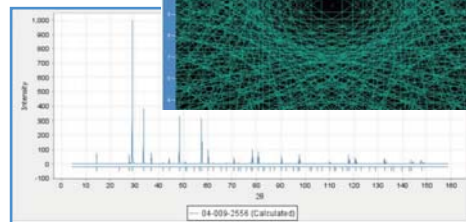
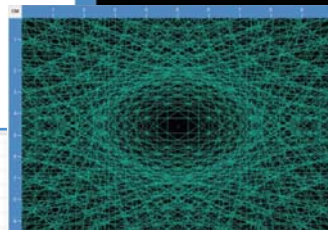
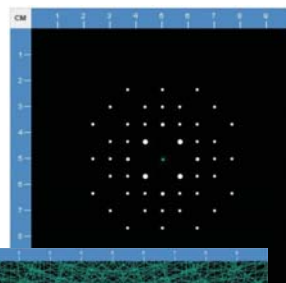
## PDF-4+, an Electron Diffraction Database

**The most comprehensive collection of inorganic powder patterns**

*Phase identification using physical, chemical and crystallographic data*

- ❖ Comprehensive materials database featuring 316,291 data sets  
*Standardized, edited data from four crystallographic databases*
- ❖ Electron diffraction simulations on >268,000 data sets  
*Interactive spot pattern display*  
*Electron diffraction backscatter pattern*
- ❖ Electron diffraction powder patterns for 316,291 data sets
- ❖ 160,183 data sets with atomic coordinates
- ❖ Atomic and molecular visualization
- ❖ Phase identification using elemental composition

*All formulas converted to both atomic and weight percentages*



**International Centre for Diffraction Data**

12 Campus Boulevard • Newtown Square, Pennsylvania 19073-3273 U.S.A.

Phone: 610.325.9814 • Toll-free: 866.378.9331 (U.S. & Canada) • Fax: 610.325.9823

[www.icdd.com](http://www.icdd.com) • [www.dxcicdd.com](http://www.dxcicdd.com)



# PDF-4+, an Electron Diffraction Database

In the 70 year history (1941–2011) of the ICDD, there have been several products developed to provide the scientific community with databases and search methods specific to the needs of electron diffraction users. While useful, prior products have struggled with the fact that most reference material data sets were based on X-ray versus electron diffraction, and the lower resolution in electron diffraction d-spacing measurements prevented fast *unique* identification of materials characteristic of X-ray methods.

PDF-4+ 2011 is an advanced product that uses simulations based on atomic structure and electron diffraction scattering. The database uses a Java™ interface and relational database format to allow the user to identify materials based on comparisons of dozens of physical, chemical and crystallographic parameters (55 searches, 91 display fields). Therefore, users can easily combine an elemental analysis with interatomic spacings or unit cell parameters. Finally, the database is comprehensive in that it contains data edited and standardized from four crystallographic databases, providing 316,291 material data sets.

## Pattern Simulations

The suite of electron diffraction tools included with the PDF-4+ database includes an electron diffraction powder pattern simulation, a spot pattern simulation and an electron diffraction backscatter pattern simulation module. The simulations are based on calculations using electron scattering from atomic parameters or electron scattering factors for >220,000 data sets and are based on X-ray scattering factors for another ~48,000 data sets. The simulations are interactive providing the user with instantaneous updating of the pattern with on-the-fly parameter changes to zone axes, camera constants, or electron voltages. There is also a provision for importing a user-collected spot image for overlaying with a simu-

lated spot pattern for visual confirmation.

## Atomic and Molecular Visualization

PDF-4+ 2011 combines four global databases derived from single crystal and powder diffraction studies. This is the fifth year where the database has combined new data from the Linus Pauling File through our collaboration effort with Material Phases Data System. This collaboration has resulted in the addition of several new materials, many published for the first time, and the addition of atomic coordinates and thermal displacement parameters. For Release 2011, the database contains 160,183 data sets with atomic parameters.

***PDF-4+ 2011 is the world's most comprehensive collection of inorganic powder patterns.***

## Key Searches

(out of 55 total search options)

<b>Powder Patterns*</b>	316,291 Entries
<b>Unit Cells</b>	285,094
<b>Citations</b>	362,335
<b>Authors</b>	116,270
<b>Atomic Coordinates</b>	160,183

\*Search by long or strong spacings

Users can perform several types of nomenclature searches, searches based on elemental composition, and searches based on author, reduced and standard cells.

PDF-4+ is available for use today. However, the ICDD considers Release 2011 to be an ongoing effort toward offering a set of powerful tools for the electron diffractionists. We are particularly interested in working with equipment manufacturers and software developers to synergistically develop interfaces between PDF-4+ and their analysis equipment and programs. Simulated data can be made even more accurate with modeling of instrumental parameters and optic configurations. Reference data, patterns, composition search results, and material physical properties can be exported from the database for use in sophisticated data analysis programs for rapid search and identification, phase mapping, modeling and structural analyses. The ICDD has such working relationships with all major manufacturers of X-ray diffraction equipment and we are seeking development partners for electron diffraction analysis.

