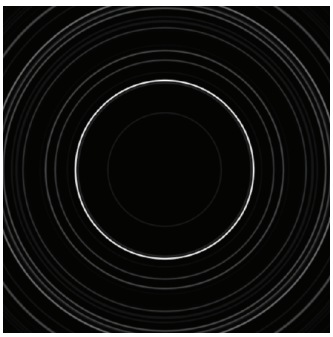
INTERNATIONAL CENTRE FOR DIFFRACTION DATA

PDF-4+ 2018

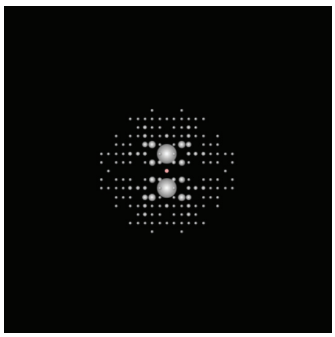
An Electron Diffraction Database

Designed for phase identification using elemental composition

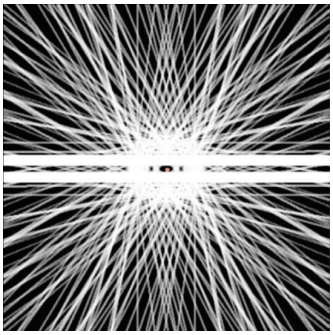
Electron diffraction simulations for 348,000+ entries



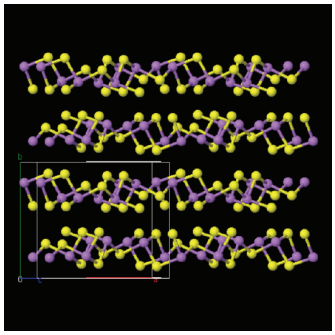
2D ring pattern



Selected area spot pattern (including indexing)



Electron backscatter diffraction pattern



Atomic and molecular visualization

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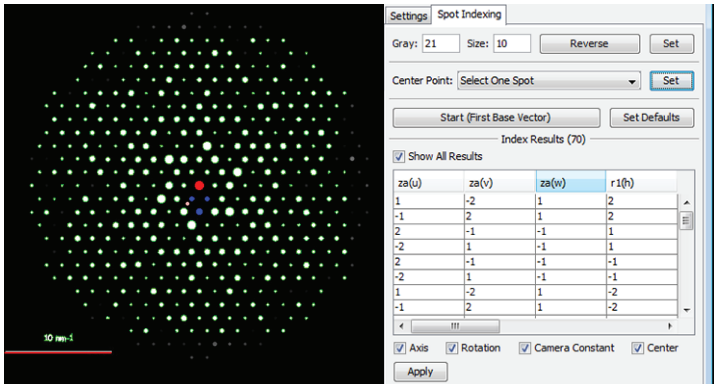
PDF-4+: An Electron Diffraction Database

Spot Pattern Indexing



PDF-4+ 2018 has the ability to index electron diffraction spot patterns collected on your instrument. Images may be imported in 'jpg', 'gif', or 'png' format. Via interactive processing, the spots in the image will be indexed based on the retrieved entry for the phase being examined.

PDF-4+ 2018 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 (72 searches, 125 display fields). Therefore, users can easily combine an elemental analyses with interatomic spacings or unit cell parameters. Finally, the database is comprehensive in that it contains data edited and standardized from five crystallographic databases, providing 398,726 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 backscatter diffraction pattern simulation. The simulations are based on calculations using electron scattering from atomic parameters, electron scattering factors, or X-ray scattering factors. The simulations are interactive providing the user with instantaneous updating of the pattern for on-the-fly parameter changes to zone axes, camera constants, or electron voltages.

Atomic and Molecular Visualization

PDF-4+ 2018 combines five global databases derived from single crystal and powder diffraction studies. Our collaboration with Material Phases Data System has resulted in the addition of new materials, many published for the first time, and the addition of atomic coordinates and thermal displacement parameters. For Release 2018, the database contains 295,309 data sets with atomic parameters.

PDF-4+ 2018 is the world's most comprehensive collection of inorganic powder patterns.

The ICDD considers Release 2018 to be an ongoing effort toward offering a set of powerful tools for the electron diffraction community. We are particularly interested in working with equipment manufacturers and software developers to 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 working relationships with all major manufacturers of X-ray diffraction equipment and we are seeking development partners for electron diffraction analysis.

ICDD® International Centre for Diffraction Data

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