STOE

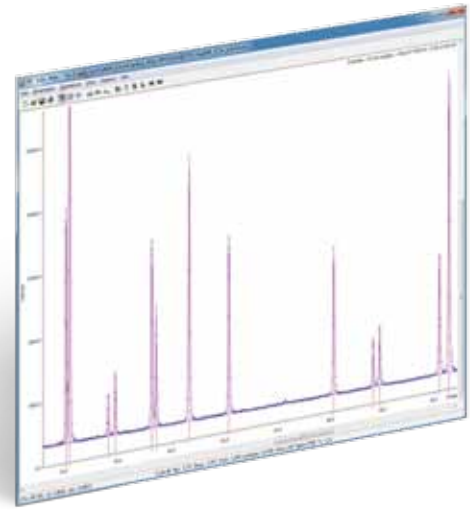
SINCE 1887



WINXPOW

POWDER DIFFRACTION SOFTWARE

THE STOE POWDER DIFFRACTION SOFTWARE PACKAGE



POWDER DIFFRACTOMETRY

WinX^{Pow} is the versatile state of the art software for controlling the high precision **STOE STADI P** diffractometer series and for data evaluation

- provides a complete package for data collection and a wide range of data evaluation
- user-friendly, modular, easy to use, yet flexible and powerful
- liberal license policy, free software update for 3 years, one license for unlimited use in your department
- CFR 21 Part 11-conform GMP package available

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POWDER DIFFRACTOMETRY

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DATA-ACQUISITION

DIFFRACTOMETER CONTROL/ TEMPERATURE CONTROL

- Versatile and intuitive interface to the STADI P diffractometer series. Easy access and control of the diffractometer and the attached equipment
- Supports a wide range of sample configurations like Transmission, Debye-Scherrer and Reflection
- For 2θ/Ω, θ/2θ, θ and Ω scans
- Automated temperature scans with several low and high temperature devices
- Measurements with sample changers can be performed directly, or executed through external programs via batch-files
- Fully automated auto-calibration: zeropoint correction within a few minutes

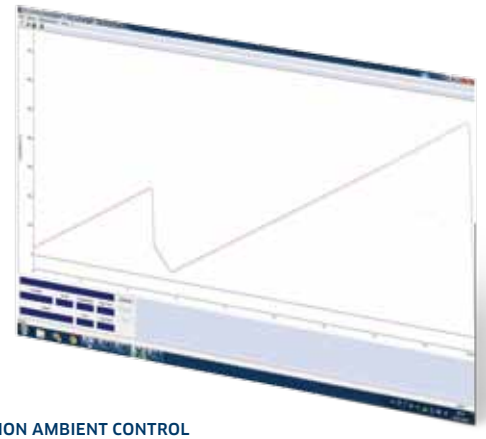
RAW DATA HANDLING

- Data reduction tools comprising background editing, absorption, dead time as well as angle correction and, if necessary, $K_{\alpha 2}$ stripping
- Complete files or selected ranges may be merged, added or subtracted
- Easy conversion of the STOE raw data format into other data formats, i.e. for importing in common Rietveld programs



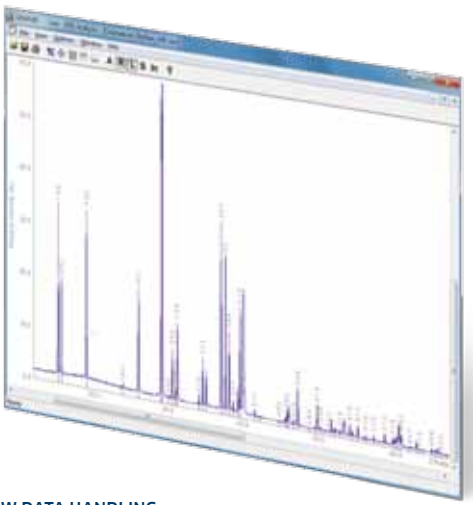
DIFFRACTOMETER CONTROL

Real-time display of measured data and diffractometer status



NON AMBIENT CONTROL

Freely definable ramp parameter control with automatic execution



RAW DATA HANDLING

Comprehensive data processing and import/export tool

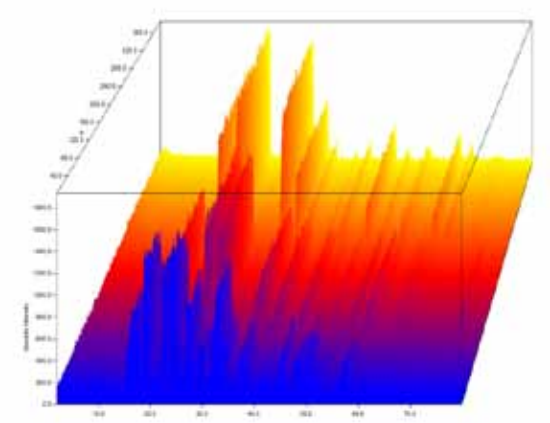
PRESENTATION

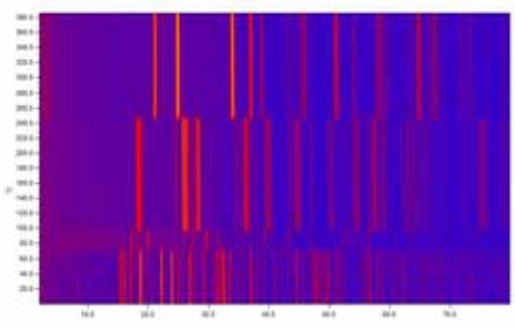
2D-GRAPHICS

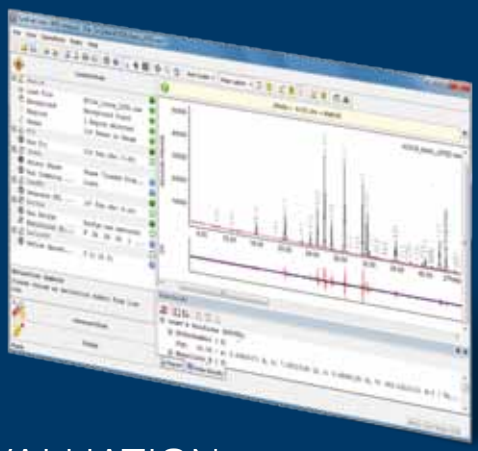
- Powerful graphics program for visualization and presentation of collected data
- Visualization of a variety of different data sets like measured data, peak data or data imported from ICDD databases
- Basic data evaluation like peak search or background editing
- All data sets are very easily arranged or labeled, with different axis scales, colors, etc.

3D-GRAPHICS

- Easily accessible 3D-Graphics visualization programm
- Flexible choice of perspective, scaling and labelling option of a 'top-down' view on a set of data curves (Guinier-plot)







EVALUATION

SYSTEVAL FOR INDEXING / CELL REFINEMENT / EXTINCTION SYMBOLS

- As pattern indexing and space group determination is often the rate limiting step in structure determination from powder data, WinX^{Pow}, with SystEval, offers a powerful tool for peak searching, indexing with three different well-known algorithms, cell refinement and determination of extinction symbols
- All performed with full pattern refinement
- Offers either a direct step by step guided way through the evaluation process, where most parameters are chosen by the program, or the expert mode, where the user has access to nearly all parameters of the algorithms
- Profile fitting and indexing also available as stand-alone modules

SIZE-STRAIN / CRYSTALLINITY

- Evaluation of size/strain measurements
- Determination of the state of crystallinity

THEORETICAL PATTERN

- Calculation of a theoretical pattern from given metric and atomic positions
- Easy import from CIF files

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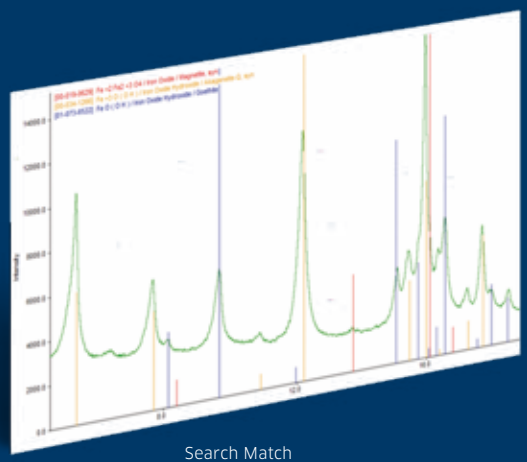
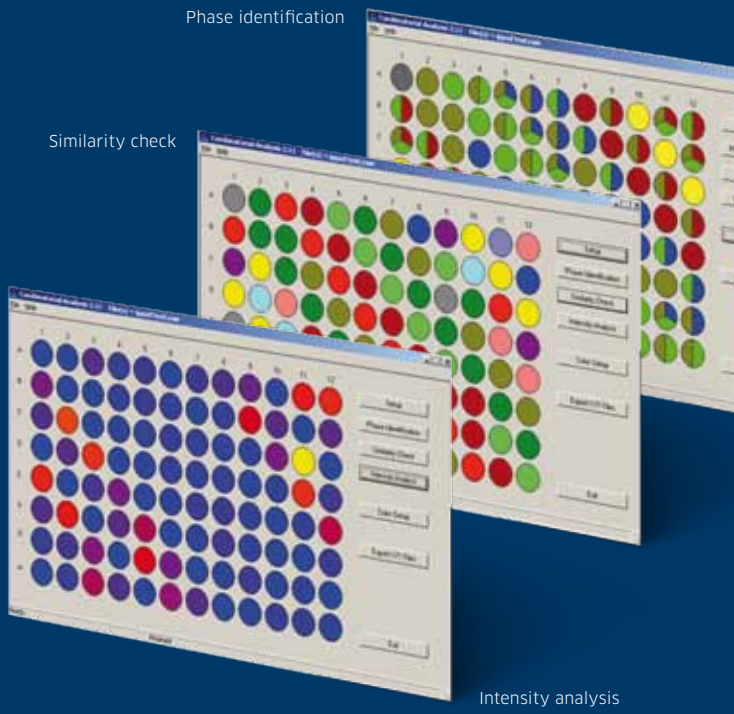


Search Match

OPTIONAL MODULES

SEARCH-MATCH

- Based on the ICDD PDF databases, phase analysis from observed powder patterns is combined with convenient database browsing
- A powerful search and match algorithm performs searches for phases of given chemical composition, mineral names or other criteria
- Semi quantitative results are calculated from the phases' tabulated I/I_{cor} values
- Database can be easily enhanced with own phases



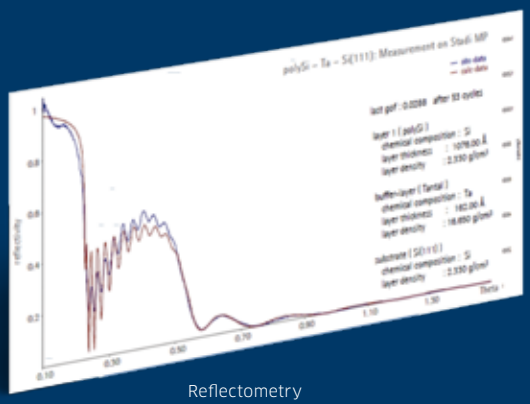
Phase identification

Similarity check

Intensity analysis

COMBINATORIAL AND HIGH-THROUGHPUT ANALYSIS

- High throughput analysis module allows phase identification, similarity checks and intensity analysis-performed on free grid of up to 96 sample wells
- Optimized graphical presentations of results by easy adjustment of parameters for each analysis



Reflectometry

REFLECTOMETRY

- The module Layer allows evaluation of thickness, density and roughness from reflectometry scans using an optimized least squares approach
- For samples of unknown composition or with unknown layers, the simulation of theoretical patterns is the first step towards identification

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