New look for Rietveld and Pawley refinement

Fully integrated with state of the art visualizer

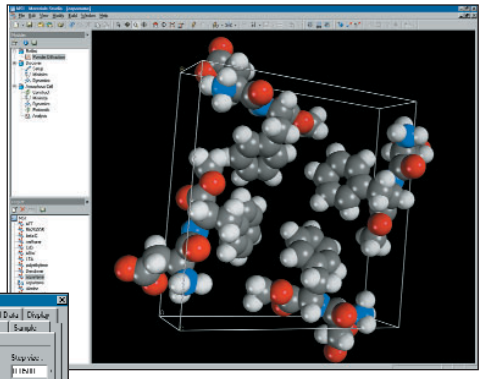
Provides interfaces to indexing programs TREOR, ITO & DICVOL

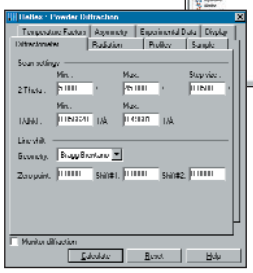
Materials Studio Datasheet

Reflex for Powder Diffraction

Reflex simulates X-ray, neutron, and electron powder diffraction patterns based on models of crystalline materials. Reflex aids the determination of crystal structure, assists the interpretation of diffraction data, and is applied to validate the results of experiment and computation.

The determination and characterization of structure is a critical step in most research projects – particularly those involving crystalline materials. Diffraction techniques, using X-rays, neutrons, or electrons, are widely employed to gain valuable information about crystals at the atomic level. Although interpretation of diffraction data can be routine for some materials, it is extremely complex for others. Whether it is at either of these extremes, or anywhere between them, the interpertation of diffraction data can use large amounts of research time.





▲ *The Materials Studio interface displaying a molecular crystal and the Reflex control panel. The predicted powder diffraction pattern for this crystal is shown overleaf.*

To accelerate this process, Reflex offers a suite of computational tools for powder diffraction simulation, powder indexing, and refinement of candidate crystal structures against experimental data. The product is fully integrated within Accelrys' Materials Studio™ software environment.

Powder Diffraction Simulation

To compute a diffraction pattern you simply construct a model of your material using the Materials Visualizer, open the Reflex Powder Diffraction dialog to choose the experimental conditions you want to simulate, and press the calculate button. Such fast, interactive simulation radically increases the efficiency of diffraction data interpretation. Feedback from simulations is graphical and easy to understand. Results can be directly compared to, and refined against, experimental data. Simulated patterns can be updated instantaneously as a structure is manipulated, allowing real-time coupling of structure modeling to experiment.

Simulations can be performed for X-rays, neutrons, and electrons. Changing diffractometer properties, the nature of the radiation, and sample parameters is straightforward – simply change the relevant values in dialog boxes that will look familiar to any user of Microsoft-compliant software.

Powder Indexing

Indexing an experimental powder pattern is often the most challenging step in determining crystal structures from powder diffraction data. Reflex provides three well known and popular indexing algorithms, TREOR90[1,2], DICVOL91[3], and ITO[4] are all available through easy to use control panels. Peak picking prior to the actual indexing run can be performed either using a choice of automatic picking methods or by choosing peaks manually.

Powder Refinement

Reflex provides two refinement methods to aid researchers in structure determination - Rietveld refinement[5,6] and modified Pawley refinement [7,8]. A new, versatile, and easy to use Rietveld refinement tool enables users to refine candidate crystal structures against experimental powder diffraction data by minimizing the weighted R-factor, R_{wp}. This factor

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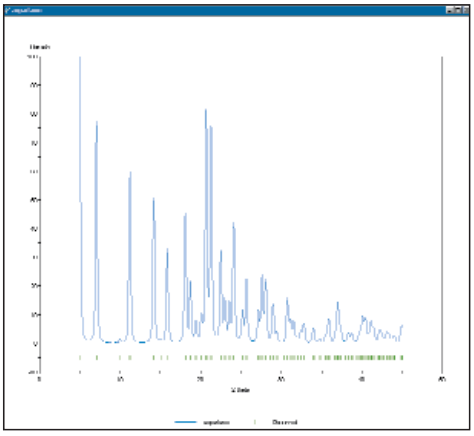
Reflex for Powder Diffraction



▲ *Powder diffraction pattern simulated with Reflex.*

describes the quality of fit between the simulated and experimental patterns. Flexibility is provided through the wide range of parameters available for refinement including lattice constrants, atomic coordinates and temperature factors, occupancies, and parameters related to the background, the zero point shift, the peak profile and asymmetry, crystallite size and lattice strain broadening, and prefered orientation. A choice of profile functions and asymmetry corrections is available.

The modified Pawley refinement tool provided within Reflex can be used to confirm indexing results and to help to explore the effect of systematic absences, aiding in the determination of possible space groups. R_{wp} is minimized independent of the atomic arrangement inside the unit cell, all peak intensities being treated as adjustable parameters. As in Rieveld refinement a wide range of variables can be refined.

The peak fitting is a two step process. In the first step the integrated intensities and background coefficients are optimized, while other parameters are fixed. In the second step, the peak shape, cell parameters, and zero-point shift are optimized for fixed values of intensities and background coefficients. The two step process can be continued until convergence is achieved.

The Materials Studio Advantage

Materials Studio's integrated model building and editing tools enable you to construct, visualize, and manipulate structures of crystalline solids. Structures that you have characterized through diffraction work are instantly available in any other Materials Studio product, and it is easy to produce high quality images. Structural information and diffraction data can readily be exported to and imported from other PC applications – allowing you to share them with colleagues and perform further analysis using spreadsheet and other packages.

Fast, efficient, integrated, and easy-to-use; Reflex provides the essential computational support for researchers investigating structure with powder diffraction.

Features

General

- Simulates powder diffraction patterns
- Supports real-time simulation during structure manipulation
- User defines the radiation wavelength and polarization
- Accounts for isotropic and anisotropic temperature factors
- Accounts for the effects of preferred orientation
- Simulates both sample and instrument broadening effects
- Indicates systematic absences
- Simulates x-ray, neutron, and electron powder diffraction data.
- Loads experimental data for direct on-screen comparison
- Provides a versatile range of peak profiles - Gaussian, Lorentz, Mod.Lorentz#1, Mod.Lorentz#2, Pseudo-Voigt, Pearson VII, Thompson-Cox-Hastings, David-Voigt, Tomandl pseudo-Voigt
- Choice of asymmetry corrections - Rietveld, Howard, Berar-Baldinozzi[9], Finger-Cox-Jephcoat[10]
- Gives optional table output of the simulated data
- Experimental data formats supported include Bruker, Stoe, Scintag, Rigaku (Jade), Philips, JCAMP, Galactic SPC, GSAS raw, ILL
- Program operated through the Materials Studio user interface on Windows® 98, NT4, Me, and 2000

Powder Indexing

- Manual or automatic peak identification
- Choice of peak search methods - simple or Savitsky Golay

- Full graphical user interface to TREOR[1,2], DICVOL[3], and ITO[4].
- Full interactivity with powder patterns and data in table format
- Choice of crystal classes to search
- Returns unit cell parameters, figure of merit
- Enables construction of unit cell from any successful solution

Powder refinement

- New refinement code, based on established and novel methods
- Choice of Rietveld[5,6] and modified Pawley[7,8] refinement methods
- Refinement of a wide range of variables - cell parameters, atomic coordinates and occupancies, temperature factors, peak profile parameters, crystallite size and lattice strain broadening, preferred orientation, background, zero-point shift, intensities
- Special positions are explicitly taken into account.
- Possibility to define motion groups (rigid bodies) with internal degrees of freedom

References

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System Details

Operated through the Material Studio users interface on Windows® 98, Me, NT4, or 2000. CPU intensive powder indexing calculations can be executed on Windows® NT4, 2000, SGI Irix, Red Hat Linux (Intel) operating systems.

Now available - Reflex Plus™, the advanced version of Reflex containing the industry leading Powder Solve technology. Reflex Plus enables complete structure determination from powder diffraction data. For details see the Reflex Plus datasheet.

Fast, efficient, integrated, and easy-to-use

Reflex provides the essential computational support for researchers investigating structure with powder diffraction

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