

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 interpretation of diffraction data can use large amounts of research time.

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's MS Modeling environment.

POWDER DIFFRACTION SIMULATION

To compute a diffraction pattern you simply construct a model of your material using 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

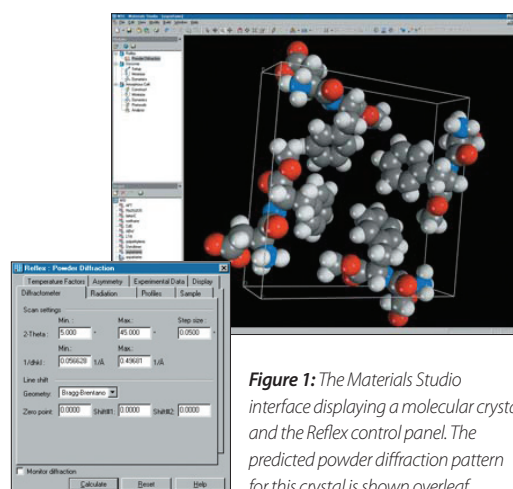


Figure 1: The Materials Studio interface displaying a molecular crystal and the Reflex control panel. The predicted powder diffraction pattern for this crystal is shown overleaf.

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.

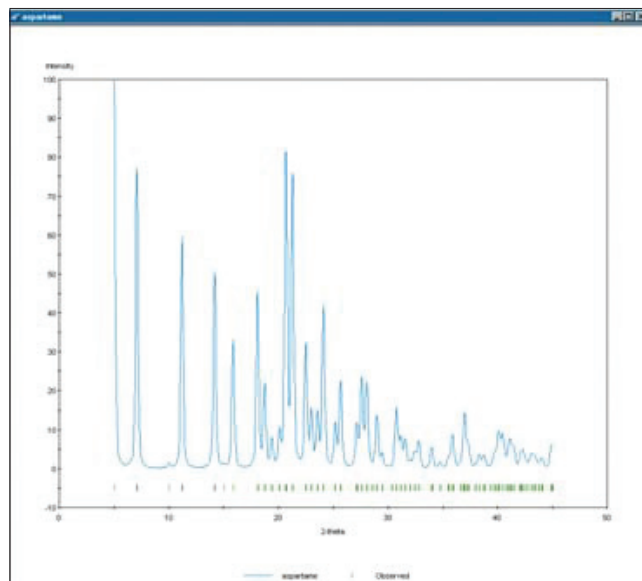


Figure 2: Powder diffraction pattern simulated with Reflex.

POWDER INDEXING

Indexing an experimental powder pattern is often the most challenging step in determining crystal structures from powder diffraction data. Reflex uses a novel indexing algorithm X-Cell¹, along with three wellknown and popular indexing algorithms, TREOR90^{2,3}, DICVOL91⁴, and ITO⁵, 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 four methods for refinement to aid researchers in structure solution - Rietveld refinement^{6,7}, Rietveld with energies, Pareto optimization⁸, and modified Pawley refinement^{9,10}. 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, Rwp. This factor describes the quality of fit between the simulated and experimental patterns. Flexibility is provided through the wide range of refinement parameters available - unit cell, atomic, peak profile and asymmetry, crystallite size and strain broadening, preferred orientation, background, zeropoint shift, intensities. Rietveld refinement with energies incorporates an accurate

description of potential energy in conjunction with Rwp during a Rietveld refinement process optimizing a combined figure of merit so that not only the simulated pattern of the resulting structure matches the experimental diffraction data, but also the potential energy of the structure is close to a global minimum. Pareto optimization can be used to calculate a set of possible optimal refinement solutions automatically as a sequence of Rietveld refinement with energies calculations with changing energy weights. Pareto optimization for a structure solution represents a trade-off to provides best possible Rwp(min) and energy(min) compromises.

The modified Pawley refinement tool provided within Reflex can be used once indexing is complete to help to explore systematic absences, aiding in the determination of possible space groups. Rwp is minimized independent of the molecular structure inside the unit cell. A wide range of variables can be refined, including a choice of peak profile and asymmetry functions, crystallite size, lattice strain, integrated Bragg intensities, and background coefficients. 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 parameters 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

Reflex is operated within the Materials Studio[®] software environment. 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, , Finger-Cox-Jephcoat
- Gives optional table output of the simulated data
- Experimental data formats supported include Bruker, Stoe, Scintag, Jade, Philips, JCAMP, Galactic SPC, GSAS raw, ILL, PAnalytical XRDML. Powder Indexing
- Data processing options includes Ka2 stripping¹¹, background subtraction¹², data smoothing, data scaling, and data interpolation
- Manual or automatic peak identification
- Choice of peak search methods - simple or Savitsky Golay
- Full graphical user interface to X-Cell1, TREOR^{2,3}, DICVOL⁴, and ITO⁵
- 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^{6,7}, Rietveld with energies, Pareto optimization⁸, and modified Pawley^{9,10} 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
- Enables automatic space group determination
- Ability to define motion groups (rigid bodies) with internal degrees of freedom.

SYSTEM DETAILS

Operated through the Materials Studio user interface on Windows® 2000 and XP. CPU intensive powder indexing calculations can be executed on Windows® 2000, 2003, XP, SGI IRIX, Red Hat (Intel IA32, Intel IA64, EM64T, and compatibles), and SuSe Linux (Intel IA32, EM64T, and compatibles), and HP Tru64 operating systems. CPU intensive powder refinement calculations can be executed on Windows 2000, 2003, XP, SGI IRIX, Red Hat Linux (Intel IA32, EM64T, and compatibles), and SuSe Linux (Intel IA32, EM64T, and compatibles) 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.

To learn more about Materials Studio, go to accelrys.com/materials-studio

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