BIOVIA MATERIALS STUDIO X-CELL

DATASHEET

BIOVIA Materials Studio X-Cell[1] is a patented, novel, robust, efficient, integrated, and easy to use indexing algorithm which uses an extinction-specific dichotomy procedure to perform an exhaustive search of parameter space to establish a complete list of all possible unit cell solutions. BIOVIA Materials Studio X-Cell provides the essential algorithmic support for researchers investigating both organic and inorganic crystal structures from medium-quality conventional laboratory powder diffraction data to high-quality synchrotron powder diffraction data obtained from X-ray, neutron, and electron radiation sources.

WHAT ARE THE CHALLENGES?

Crystal structure determination frequently is a prerequisite for the rational understanding of the solid-state properties of new materials. The ideal method for solving crystal structures is through single-crystal X-ray diffraction. Growing single crystals of appropriate size, however, is often difficult or even impossible, whereas powder samples are readily available for analysis by powder diffractometry. Indexing the experimental powder pattern has emerged as a significant bottleneck for crystal structure determination from powder diffraction data.

The failure rate of the commonly used indexing algorithms is fairly high. Most indexing programs do not determine the zero-point shift of the powder diffraction pattern together with the unit cell parameters, that may prevent the success of the search for unit cell parameters. The robustness with respect to impurity peaks is, in general, fairly low, and none of the existing programs offers a choice of specific impurity tolerance levels. Indexing a flat unit cell is a particular challenge, since all or most of the selected reflections may belong to the dominant zone in reciprocal space, and the unit cell may not be uniquely defined.A high ratio of reflections may not be observed due to peak overlap, preferred orientation, or poor statistics. In such cases, the correct unit cell is difficult to distinguish from the large number of incorrect solutions with similar figures of merit.

WHAT DOES BIOVIA MATERIALS STUDIO X-CELL DO?

Developed at Accelrys, BIOVIA Materials Studio X-Cell is an innovative indexing algorithm that addresses many of the shortcomings of conventional indexing algorithms. By taking into account systematic absences during the search, the ability to identify the correct indexing solution is greatly enhanced.

The volume of parameter space and the number of incorrect solutions increase rapidly with the number of calculated peaks. BIOVIA Materials Studio X-Cell performs a search from low to high peak numbers while explicitly taking into account systematic absences.

The correct unit cell is therefore found earlier and thus reduces the required CPU time. In addition, the correct unit cell is less likely to be hidden among a large number of incorrect solutions.

BIOVIA Materials Studio X-Cell is the first indexing program to use explicit impurity tolerance levels to specify the maximum number of unindexed reflections among the experimentally observed reflections. Correct unit cells can be found even in the presence of impurity contamination in a main crystalline phase, a task that is very difficult if not impossible for current indexing programs. In some cases, the dominant phase of mixtures can be indexed in the presence of even up to 50% impurity peaks if high-quality synchrotron data are available.

For a given range of allowed calculated peak numbers, a given pattern of systematic absences, and a given impurity tolerance level, an exhaustive search is performed using a successive dichotomy procedure. Zeropoint shift is determined along with unit cell parameters. All indexing solutions are fully optimized, compared, and ranked according to a relative figure of merit Fr. Fr favors solutions with low numbers of calculated peaks, adjustable parameters, and impurity peaks. Indexing of long and flat unit cells is facilitated by the ability to search for rows (1D) or zones (2D) in reciprocal space first, and then the search is refined using the lattice parameters of the dominant row or zone in the final unit cell (3D) search in combination with a modified Pawley refinement[2].

The main advantages of BIOVIA Materials Studio X-Cell are completeness and robustness. Regardless of whether or not a promising unit cell has already been found, the algorithm continues to search larger and larger portions of parameter space until the search is complete or interrupted by the user. Initial validation1 indicated that BIOVIA Materials Studio X-Cell has a higher success rate (92%) than DICVOL[3] (46%), TREOR[4] (46%), and ITO[5] (33%) for 24 representative cases. BIOVIA Materials Studio X-Cell copes very well with various difficulties that are typically encountered in powder indexing, including contamination with impurity phases, strong peak overlap, peak position errors, zero-point shift and extreme cell geometries. Implementation of the successive dichotomy approach is significantly more efficient in BIOVIA Materials Studio X-Cell than in DICVOL[3].

THE BIOVIA MATERIAL STUDIO ADVANTAGE

BIOVIA Materials Studio X-Cell is implemented in BIOVIA Materials Studio Reflex, operated within the BIOVIA Materials Studio® software environment. BIOVIA Materials Studio's integrated model building and editing tools enable you to construct, visualize, and manipulate structures of crystalline solids (e.g., drugs, pigments, metals, metal oxides, zeolites, etc.) using BIOVIA Materials Studio Visualizer. Results obtained by indexing are readily passed on to other modules in BIOVIA Materials Studio Reflex and BIOVIA Materials Studio Reflex Plus for a full structure solution determination. It is easy to produce high quality images. Structural information and diffraction data can be readily exported to and imported from other PC applications - allowing you to share them with colleagues and perform further analysis using a spreadsheet and other packages.

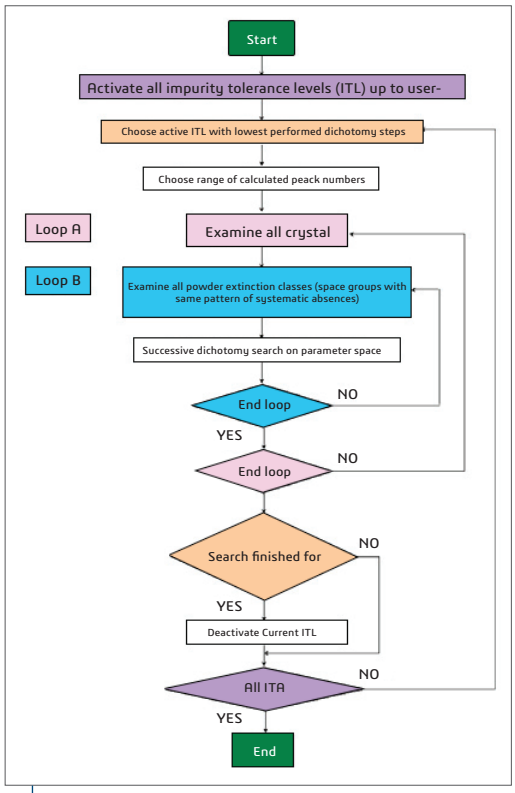

Diagram 1: Workflow of BIOVIA Materials Studio X-Cell

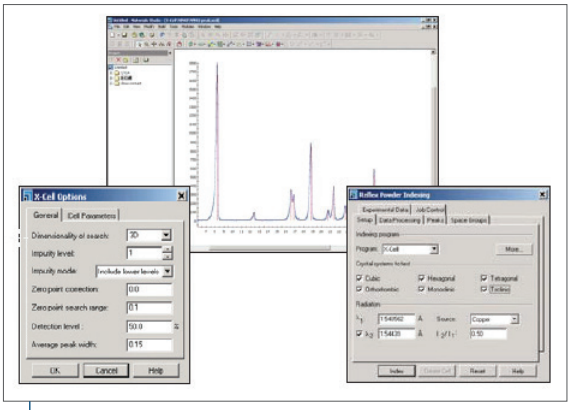

Figure 1: The BIOVIA Materials Studio interface displaying an experimental X-ray powder diffraction pattern and the BIOVIA Materials Studio X-Cell control panel

HOW DOES BIOVIA MATERIALS STUDIO X-CELL WORK?

The task of indexing involves finding a unit cell for which the calculated 2θ positions of the diffraction peaks match the experimentally observed peak positions. Diagram 11 illustrates the workflow of BIOVIA Materials Studio X-Cell. An example of inputs for BIOVIA Materials Studio X-Cell calculations is shown in Figure 1. The correctness of a unit cell solution can be verified easily through a Modified Pawley Refinement as indicated in Figure 2.

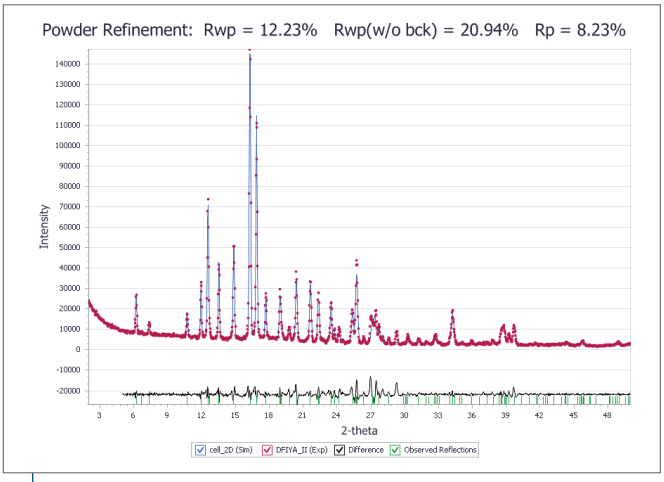

Figure 2: Correct unit cell obtained from BIOVIA Materials Studio X-Cell confirmed with a Modified Pawley Refinement

FEATURES

- Reads in a variety of diffractometer file formats including Bruker, Stoe, Scintag, Jade, Philips, JCAMP, Galactic SPC, GSAS raw, ILL, PAnalytical XRDML
- Allows for different X-ray sources with arbitrary wavelengths.
- Suitable for X-ray, neutron, and electron diffraction
- Ability to pre-process experimental data, for example via background subtractions, data interpolation, data smoothing, data scaling, and Ka2 strippings
- Manual or automatic peak identification
- Choice of peak search methods - simple or Savitsky Golay
- Choice of dimensionality search on rows (1D), zones (2D), and unit cell (3D)
- Eight different impurity tolerance levels control allowable impurity peaks among the experimentally observed peaks
- Two impurity modes to enable searches at an allowed impurity tolerance level only, or in parallel at all impurity levels up to the allowed maximum
- Can handle any possible space group, both standard and nonstandard settings, accounting for systematic absences
- Controls the bounds of the search dimension by setting target values and allowed errors for one or three lattice parameters
- User-defined highest allowed number of calculated peaks
- Ability to set expected zero-point shift and the range for the zero-point search
- Full interactivity with powder pattern and data in table format
- Returns unit cell parameters, figures of merit, a stability parameter,number of impurity peaks,number of observed peaks, number of calculated peaks not overlapped with observed peaks, zero-point shift, average 2θ deviations trial

- Enables construction of a unit cell from any successful solution, for further analysis with BIOVIA Materials Studio Reflex tools
- Benefits from straightforward interaction with other BIOVIA Materials Studio products as well as other PC applications

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