



iPowder: advanced software for automated high-throughput X-ray diffraction analysis

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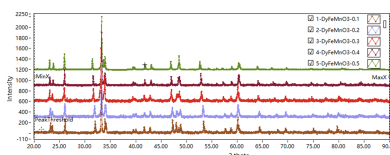
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In the burgeoning era of materials genomics, the need for fast and accurate X-ray diffraction (XRD) analysis has never been greater. To accommodate the rapid data generation of high-throughput XRD experiments, a new and powerful computer program, *iPowder*, has been developed. Not only does it have an efficient and straightforward graphical user interface but it also excels in high-throughput data analysis. The main function of the program is the rapid processing of datasets. This paper presents the convenient functionalities provided by *iPowder* for high-throughput XRD data analysis.

1. Introduction

In 2011, the United States proposed the Materials Genome Initiative (MGI). In contrast to the traditional 'trial-and-error' model of research and development, MGI accelerates the discovery of new materials through materials big data, significantly improving the efficiency of new materials research. In the materials field, high-throughput experimental technology refers to the preparation and characterization of a large number of samples in a short period of time, which means that a large amount of data needs to be processed and analyzed simultaneously. This approach is a critical component in building large materials databases, offering promising prospects in areas such as thermoelectric materials (Deng *et al.*, 2024), high-entropy alloys and lithium-ion batteries (Zhang *et al.*, 2022). X-ray diffraction (XRD), a common method for characterizing the structural features of crystalline materials, has also been extensively studied in high-throughput applications. For example, Wang *et al.* (2022) demonstrated the effectiveness of two-dimensional energy-dispersive X-ray diffraction as a high-throughput material characterization technique using white light and a simulated energy-dispersive array detector. Furthermore, the rapid development of synchrotrons has significantly increased the speed of XRD experiments and the amount of raw data collected during each experiment (Wang *et al.*, 2018). The advancement of high-throughput XRD characterization techniques necessitates the development of high-throughput XRD data analysis software capable of highly automated multi-file analysis.

It is well known that the first step in determining the crystal structure of an unknown phase is to identify the unit cell and its lattice constants. This process, known as 'indexing', often involves assigning Miller indices (*hkl*) to the diffraction peaks.



With the advancement of computer technology, several classic command-line indexing programs have emerged, such as *Dicvol* (Louër & Boulton, 2006), *Treor* (Werner *et al.*, 1985), *Ito* (Visser, 1969) and *McMaille* (Le Bail, 2004). Each of these indexing software programs has different principles and features. Some experts believe that comparing the results of different software can help to identify the correct lattice. In addition, new programs have introduced graphical user interfaces (GUIs) for these command-line tools, such as *Crysfire2020* (Ron Ghosh & Epsom, 2024) and *PowderX* (Dong, 1999). *Crysfire2020* integrates eight different indexing programs to improve the probability of finding the correct cell parameters. It only requires a set of diffraction peak positions as input, which is very convenient for users, although it requires additional peak-searching software. With a light-weight and convenient graphical interface, *PowderX* performs data processing operations with several novel algorithms and uses *Treor* for indexing.

The approximate unit-cell parameters provided by the indexing results must be refined. Essentially, this refinement process is a least-squares fitting procedure that allows accurate determination of small changes in unit-cell parameters for a set of XRD patterns obtained under varying temperature, pressure or other conditions.

iPowder has been developed to facilitate the rapid processing of high-throughput XRD experimental data, allowing automated indexing and unit-cell refinement for multiple XRD patterns. The program also integrates the phase analysis capabilities from the previously released *iQual* (Lv *et al.*, 2024), further enhancing its functionality and making it adaptable to various applications. Overall, the program offers the following key features: (a) a highly user-friendly GUI, as

illustrated in Fig. 1; (b) various data processing capabilities, such as background removal, smoothing and $K\alpha_2$ removal; (c) reliable phase analysis based on a new database and novel search-matching methods; (d) integration of the indexing programs *Dicvol06*, *Treor90*, *Ito15* and *McMaille-v4*, allowing for highly automated indexing solutions; (e) the inclusion of symmetry constraints and consideration of systematic errors during unit-cell parameter refinement, with the ability to continuously refine a series of XRD patterns; (f) full batch processing capabilities, ideal for high-throughput data analysis.

2. Features and functions

The *iPowder* program features a GUI designed using *LabView*, while the internal processing code is written in Python. This combination leverages the strengths of *LabView* in graphical programming and rapid prototyping, as well as the robust capabilities of Python in data processing, scientific computing and scripting. This architecture enables the software to provide both intuitive user interaction and efficient handling of complex algorithms and large datasets. The features and capabilities of *iPowder* are detailed below:

(i) Data import. The program is capable of intelligently importing various types of data files without needing to know the specific format of the data beforehand. This feature allows for flexible and seamless integration of data from different sources, enhancing the versatility and user-friendliness of the software. In addition, the program can recognize Crystallographic Information Framework (CIF) files, and compute simulated XRD data based on the crystal structure information using code adapted from *FullProf* (Rodríguez-Carvajal, 1993). Importantly, this program allows the simultaneous

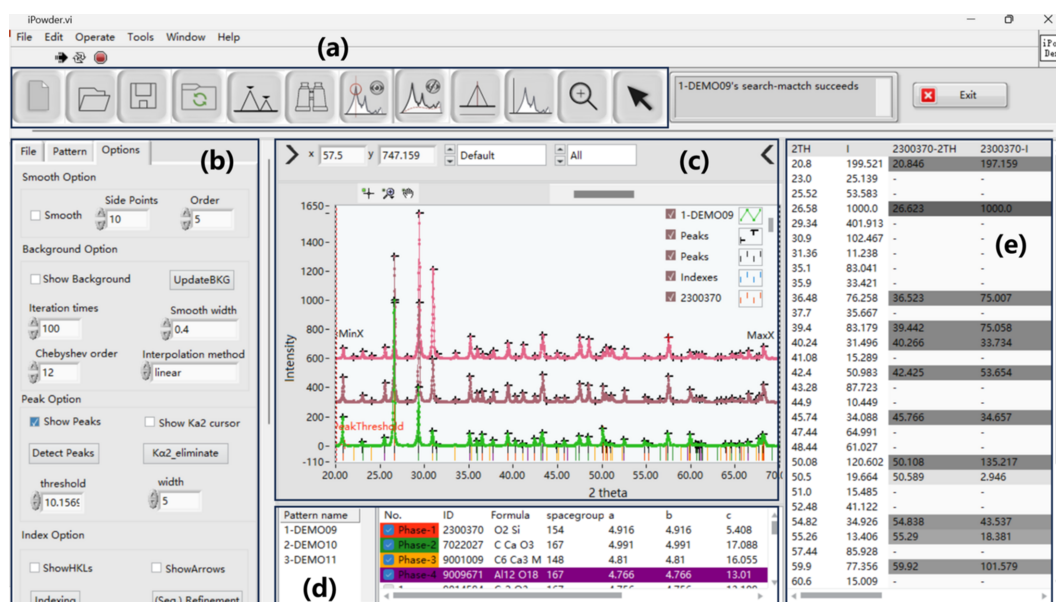


Figure 1
iPowder program interface and search-matching functionality. (a) to (e) illustrate the functional sections within the *iPowder* program: (a) quick access toolbar; (b) operations panel, including file import, pattern control and option selection; (c) pattern display area; (d) results display area; and (e) peak position display area. The figure also shows the search-matching functionality of the *iPowder* program. In (c), the XRD patterns are displayed from bottom to top as DEMO09, DEMO10 and DEMO11, and partial search-matching results are shown in (d).

import of multiple XRD patterns and CIF files, making it well suited for high-throughput data analysis. Diffraction intensities are automatically normalized during the import process, allowing users to focus on the diffraction peak positions.

(ii) Data management. To handle the large amount of data involved in high-throughput data analysis, the program provides an effective data management platform through a well designed user interface. This platform organizes and manages different types of data in different GUI sections, as shown in Fig. 1. Imported XRD patterns are displayed in section (c), while related information management and settings are found under the 'Pattern' tab in section (b). Search-matching or peak-indexing information is displayed in sections (d) and (e), with section (d) listing all possible results for each pattern and section (e) providing detailed peak-matching or peak-indexing information with a specific result from (d). This streamlined pattern management and clear display of results allows users to focus on data processing and results analysis, improving the overall user experience.

(iii) Data preprocessing. The program can quickly perform various data preprocessing tasks on multiple spectra, such as background removal, $K\alpha_2$ stripping, data smoothing and peak finding. The program uses the Brückner method (Brückner, 2000) to fit and remove the background. Users can also manually edit background points if necessary. The program uses the Savitzky–Golay method (Savitzky & Golay, 1964) and Dong's method (Dong, Chen *et al.*, 1999) to implement data smoothing and $K\alpha_2$ stripping, respectively. The program uses the *LabView* tool library for automatic peak finding but also allows the user to manually add or remove peaks.

(iv) Search-matching. The program supports fast and efficient batch phase analysis of multiple XRD patterns, greatly improving the efficiency of phase identification. It utilizes a newly developed database called *Crystal_db*, in conjunction with an innovative search-match algorithm, which expands the scope of queries and improves search efficiency. Both the database and the algorithm introduced in previous publications have been adapted in this program for high-throughput data analysis. In addition, once the qualitative and semi-quantitative phase analysis has been carried out, the program can download the corresponding CIF files from the Crystallography Open Database (COD; Gražulis *et al.*, 2009). These files can be used as a starting local database for the newly developed *FullProfAPP* (Arcelus *et al.*, 2024), which is able to perform a full Rietveld refinement in an automatic mode, improving the quantitative phase analysis.

(v) Indexing. To improve the accuracy of indexing, the program integrates four freely available indexing programs: *Dicvol06*, *Treor90*, *Ito15* and *McMaille-v4*. These programs are from the *FullProf Suite* and can automatically generate PCR files after indexing to enhance the interoperability of *iPowder* with the *FullProf Suite*. The *iPowder* program allows multiple diffraction patterns to be indexed simultaneously with a single task submission, greatly increasing analysis efficiency. For each pattern, the program can apply user-selected indexing programs, increasing the likelihood of obtaining accurate results. Extensive preprocessing is also performed,

allowing users to operate these indexing programs without having to understand their computational parameters. Users only need to decide which programs to use and which crystal system to calculate for the indexing task, greatly simplifying the process and making it highly accessible to non-specialists. Each possible solution is displayed below the XRD pattern, consisting of figure of merit, unit-cell parameters, zero shift and so on. When a particular solution is selected, the corresponding *hkl* for each observed peak is annotated on the pattern, with detailed information displayed on the right.

(vi) Unit-cell refinement. The program can refine the unit-cell parameters obtained from indexing calculations. More importantly, for a set of XRD spectra where the crystal structure remains unchanged and only the unit-cell parameters exhibit slight variations, the program can perform sequential refinement based on known approximate values. This eliminates the need for multiple complex Rietveld refinements, significantly reducing the time required to obtain accurate unit-cell parameters in such cases and thereby improving analysis efficiency. In the presence of systematic errors, assumed here to be the zero shift and sample-height displacement parameters, the program can also refine them; details of the implementation are discussed in the following section. The user can choose whether to refine the zero shift or the sample-height displacement parameters.

3. Indexing and unit-cell refinement methods

As mentioned above, the detailed algorithms for search-matching and phase analysis have been thoroughly discussed in previous publications. Therefore, this section will focus primarily on the specific methods used for indexing and unit-cell refinement.

During indexing, *iPowder* automatically constructs input files for the following programs: *Dicvol06*, *Treor90*, *Ito15* and *McMaille-v4*, allowing them to run in default mode. For each potential result, the software completes the Miller indices of all observed peaks based on their lattice parameters, since not all indexing programs assign *hkl* to all observed peaks. In addition, the program uses the refined Dong diffraction-pair method (Dong, Wu *et al.*, 1999) to calculate the zero shift. Unlike the Dong method, which uses the diffraction-pair method to determine zero shift before indexing, *iPowder* applies the diffraction-pair method after the indexing process. In addition, when multiple diffraction pairs are present, the pair that minimizes the sum of the squared differences between the corrected and calculated positions of all observed peaks is selected.

After indexing, the program uses the gradient descent method, iterating the lattice parameters to minimize the sum of squared differences between the calculated and observed peak positions. The gradient is computed using the finite difference method. During the refinement process, symmetry constraints are taken into account to preserve the crystal system. When systematic errors are introduced, the program uses the alternating least-squares (ALS) method for refinement, which alternates between refining the unit-cell

	Pattern name	No.	ID	Formula	spacegroup	a	b	c	Scale	FOM	RIR	W.T.%
(a)	1-DEMO09	Phase-1	2300370	O ₂ Si	154	4.916	4.916	5.408	1.0	0.815	4.271	53.463%
	2-DEMO10	Phase-2	7022027	C Ca O ₃	167	4.991	4.991	17.088	0.402	0.774	3.249	28.252%
	3-DEMO11	Phase-3	9001005	C ₆ Ca ₃ M	148	4.81	4.81	16.055	0.102	0.747	2.525	9.224%
		Phase-4	9009671	Al ₁₂ O ₁₈	167	4.766	4.766	13.01	0.04	0.849	1.008	9.061%
	Pattern name	No.	ID	Formula	spacegroup	a	b	c	Scale	FOM	RIR	W.T.%
(b)	1-DEMO09	Phase-1	1011172	O ₂ Si	152	4.913	4.913	5.405	1.0	0.785	4.255	35.685%
	2-DEMO10	Phase-2	2100992	C Ca O ₃	167	4.991	4.991	17.062	0.685	0.786	3.237	32.131%
	3-DEMO11	Phase-3	9001043	C ₆ Ca ₃ M	148	4.811	4.811	16.047	0.297	0.809	2.523	17.874%
		Phase-4	9009671	Al ₁₂ O ₁₈	167	4.766	4.766	13.01	0.095	0.818	1.008	14.310%
	Pattern name	No.	ID	Formula	spacegroup	a	b	c	Scale	FOM	RIR	W.T.%
(c)	1-DEMO09	Phase-1	1538064	O ₂ Si	154	4.913	4.913	5.405	0.384	0.737	3.218	15.277%
	2-DEMO10	Phase-2	1547350	C Ca O ₃	167	4.988	4.988	17.057	1.0	0.765	3.283	38.996%
	3-DEMO11	Phase-3	9001415	C ₆ Ca ₃ M	148	4.806	4.806	16.006	0.612	0.806	2.504	31.290%
		Phase-4	9009783	Al ₄ O ₆	167	5.12	5.12	5.12	0.113	0.796	1.002	14.438%

Figure 2

Detailed results of search-matching. (a) to (c) display the phase analysis results for DEMO09, DEMO10 and DEMO11, respectively.

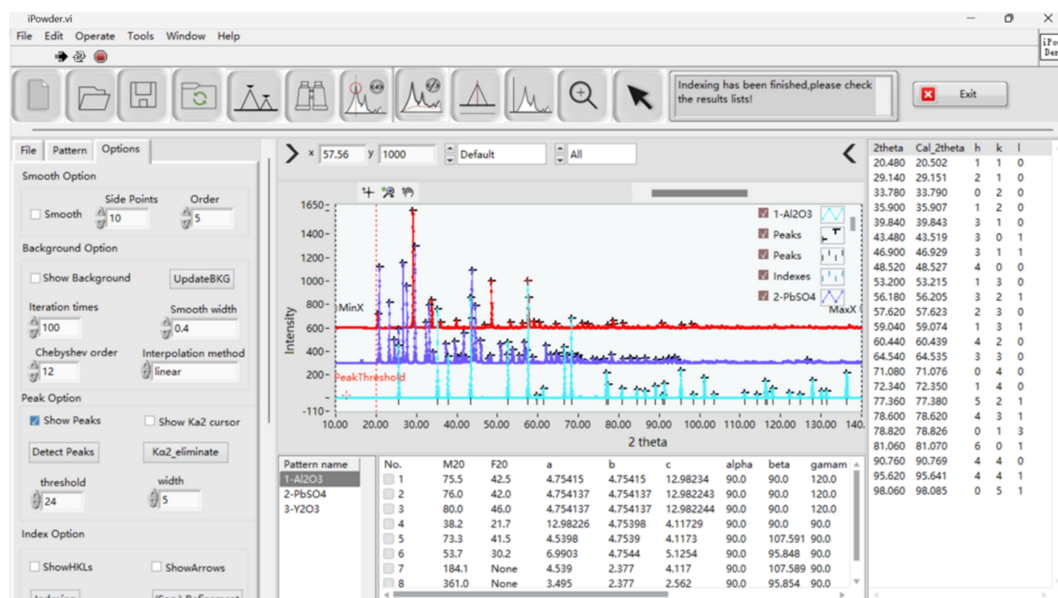


Figure 3

Demonstration of indexing functionality. The XRD patterns displayed in the figure, from bottom to top, are Al₂O₃, PbSO₄ and Y₂O₃.

	Pattern name	No.	M20	F20	a	b	c	alpha	beta	gamma	Program	Crystal system	Zeroshift	Displayment
(a)	1-Al2O3	1	78.1	49.7	4.75426	4.75426	12.98244	90.0	90.0	120.0	DICVOL06	Hexagonal	-0.00457867	
	2-PbSO4	2	85.0	55.0	4.754158	4.754158	12.982124	90.0	90.0	120.0	TREOR90	Hexagonal	-0.00280597	
	3-Y2O3	3	81.0	53.0	4.75416	4.75416	12.982129	90.0	90.0	120.0	TREOR90	Hexagonal	-0.00280597	
		4	175.66	111.43	4.754	4.754	12.9806	90.0	90.0	120.0	McMille	Hexagonal	0.003337669	
		5	38.1	24.1	12.98295	4.75412	4.11745	90.0	90.0	90.0	DICVOL06	Orthorhombic	-0.00457867	
	Pattern name	No.	M20	F20	a	b	c	alpha	beta	gamma	Program	Crystal system	Zeroshift	Displayment
(b)	1-Al2O3	1	56.5	73.3	8.48032	6.96163	5.39927	90.0	90.0	90.0	DICVOL06	Orthorhombic	0.033146372	
	2-PbSO4	2	31.0	39.0	8.485304	6.96452	5.401419	90.0	90.0	90.0	TREOR90	Orthorhombic	-0.01123452	
	3-Y2O3	3	31.0	39.0	8.485304	6.96452	5.401419	90.0	90.0	90.0	TREOR90	Orthorhombic	-0.01123452	
		4	59.7	None	6.96	8.478	5.398	90.0	90.0	90.0	ITO13	Orthorhombic	0.053735083	
		5	38.2	None	10.794	13.92	8.477	90.0	90.0	90.0	ITO13	Orthorhombic	0.053735083	
		6	5.1	None	15.212	19.6	12.064	90.0	90.0	90.0	ITO13	Orthorhombic	0.053735083	
		7	8.8	None	12.044	12.103	12.002	90.0	90.0	90.0	ITO13	Orthorhombic	-0.01944795	
	Pattern name	No.	M20	F20	a	b	c	alpha	beta	gamma	Program	Crystal system	Zeroshift	Displayment
(c)	1-Al2O3	1	65.9	58.2	10.6008	10.6008	10.6008	90.0	90.0	90.0	DICVOL06	Cubic	0.018611656	
	2-PbSO4	2	63.0	56.0	10.602761	10.602761	10.602761	90.0	90.0	90.0	TREOR90	Cubic	0	
	3-Y2O3	3	64.0	59.0	10.602765	10.602765	10.602765	90.0	90.0	90.0	TREOR90	Cubic	0	
		4	68.5	61.34	10.605	10.605	10.605	90.0	90.0	90.0	McMille	Cubic	-0.00993700	
		5	129.4	117.1	7.49428	7.49428	5.30078	90.0	90.0	90.0	DICVOL06	Tetragonal	0.024581855	
		6	60.1	None	7.494	7.494	5.299	90.0	90.0	90.0	ITO13	Tetragonal	0.042020108	
		7	82.2	None	5.299	7.494	5.299	90.0	90.0	90.0	ITO13	Tetragonal	0.042020108	
		8	101.6	92.3	7.4931	5.29981	3.74808	90.0	90.0	90.0	DICVOL06	Orthorhombic	0.024581855	

Figure 4

Detailed indexing results. (a) shows the indexing results for Al₂O₃, with 1, 2 and 3 being the correct results. (b) presents the indexing results for PbSO₄, with 5 being the correct result. (c) displays the indexing results for Y₂O₃, with 1 and 2 being the correct results.

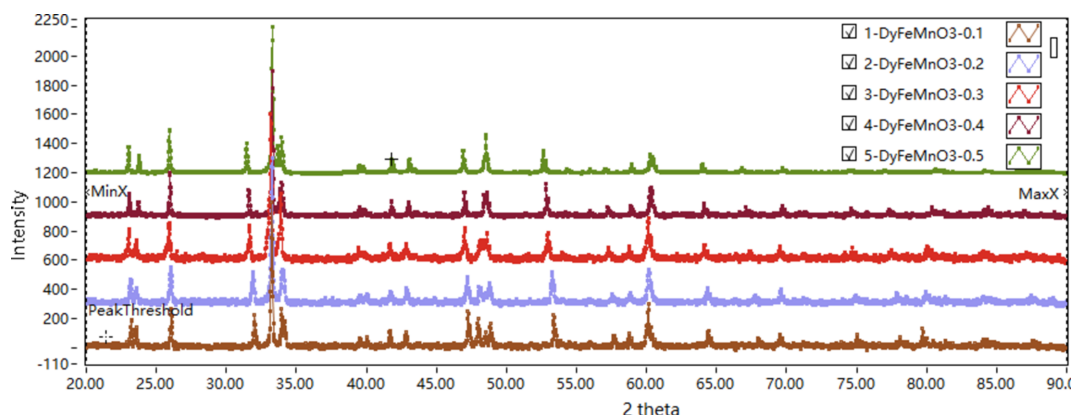


Figure 5
The XRD patterns with Mn ions substituted into Fe sites of DyFeO_3 in 10%–50% ratios.

parameters, zero shift and sample-height displacement in a stepwise manner, ensuring each is optimized for accurate results. The zero shift should ideally be calibrated with a standard sample or alternatively calculated using the improved Dong method mentioned above. If neither calibration with a standard sample nor the Dong method is available or effective, zero shift refinement can be used as an alternative to estimate the zero shift value during lattice parameter refinement. Sample-height displacement affects diffraction peak positions according to the formula $\Delta 2\theta = -2.0 \times \text{dis} \times \cos(\theta)$, where *dis* is the sample-height deviation from its standard value. The ALS method is based on the previously discussed gradient descent technique, and by selecting different iteration parameters according to the refinement objectives, this method can be effectively implemented.

4. Examples

4.1. Search–matching

Three diffraction patterns – DEMO09, DEMO10 and DEMO11 – each containing SiO_2 , Al_2O_3 , CaCO_3 and $\text{CaMg}(\text{CO}_3)_2$ in different proportions, were used to demonstrate the batch search–matching function. The patterns and performance of *iPowder* are shown in Fig. 1. Detailed phase analysis results for each diffraction pattern are shown in Fig. 2, including the specific weight fraction of the different phases.

4.2. Indexing

To demonstrate the indexing performance of *iPowder*, three diffraction patterns (Al_2O_3 , PbSO_4 and Y_2O_3) with different crystal systems were used, as detailed in Table 1. The *iPowder* software was employed to index these diffraction patterns simultaneously, as depicted in Fig. 3, demonstrating the software's ability to handle batch data processing efficiently. The detailed indexing results for each pattern are displayed in Fig. 4, which quickly provides the correct indexing results compared to the information in Table 1.

4.3. Unit-cell refinement

The application of *iPowder* in sequential unit-cell refinement is illustrated by a series of experimental XRD patterns

where Mn ions have been substituted into Fe sites of DyFeO_3 at ratios of 10%–50%, as described in a previous article (Yang *et al.*, 2024). Fig. 5 shows the XRD patterns of this material, with Mn ion occupancy ratios of 10%, 20%, 30%, 40% and 50% from bottom to top. The *iPowder* program was used to select diffraction peaks corresponding to the calculated diffraction lines for the refinement of unit-cell parameters, with initial parameters obtained from the referenced article. The variations of the refined unit-cell parameters are shown in Fig. 6, where it is evident that only the *a*, *b* and *c* axes were refined due to symmetry constraints. The results show that the lengths of the *a* and *c* axes decrease, while the length of the *b* axis increases with increasing Mn occupancy.

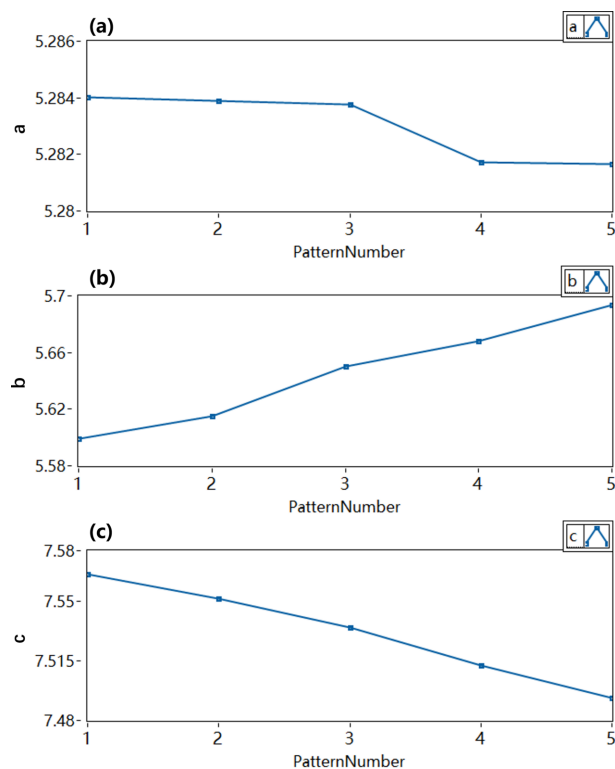


Figure 6
Results of unit-cell parameter refinement. Panels (a) to (c) display the variations in the unit-cell axes *a*, *b* and *c*, respectively.

Table 1

Details of crystal systems used to demonstrate indexing performance.

Al_2O_3 was obtained from COD, with CIF file numbered 2101054, and its diffraction pattern was calculated using the *FullProf* software (Rodríguez-Carvajal, 1993). PbSO_4 and Y_2O_3 diffraction patterns were collected with the Bruker D8 Advance instrument. The correct cell parameters for these three materials are also shown here

Pattern	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	α (°)	β (°)	γ (°)	Radiation	Source
Al_2O_3	4.754	4.754	12.982	90	90	120	Cu $K\alpha_1$	Calculation
PbSO_4	6.960	8.480	5.399	90	90	90	Cu $K\alpha_1$ and $K\alpha_2$	Experiment
Y_2O_3	10.600	10.600	10.600	90	90	90	Cu $K\alpha_1$ and $K\alpha_2$	Experiment

5. Conclusion

These examples not only illustrate the application of *iPowder* in search–matching, indexing and sequential unit-cell refinement but also demonstrate the program's automation capabilities and robust data processing features. In addition, *iPowder* has an easy-to-use and concise GUI that allows for easy batch processing, making it ideal for high-throughput XRD experiments. They have been thoroughly verified and they differentiate *iPowder* from previously released software. In the future, *iPowder* will incorporate more functionalities, such as crystal structure determination and automated Rietveld refinement by linking with *FullProfAPP*, building on the initial phase analysis results to streamline comprehensive quantitative refinement. Ultimately, it will evolve into a comprehensive software package for XRD full-process analysis, providing greater convenience and efficiency for researchers.

6. Distribution

iPowder can be downloaded from <https://github.com/iPowder/iPowder>. *iPowder* is compatible with Windows 10/11 systems. *iPowder* is released free of charge for academic purposes. Commercial users must pay a fee. Questions about the program may be addressed to the authors by email (fengzhenjie@shu.edu.cn, changshihui@shu.edu.cn or whitestar@shu.edu.cn).

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