Development of a graphical user interface for visualizing solid-state crystal parameters from XRD data and the Cramer-Cohen algorithm for sustainable material management

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Abstract. Accurate characterization of crystalline materials is critical for advancing low-carbon energy systems, pollution remediation, and sustainable infrastructure—applications where structural precision directly impacts environmental and economic sustainability. This study introduces a Python-based GUI tool that streamlines lattice parameter calculations by integrating the Cramer-Cohen algorithm, which applies Bragg's law and crystallographic geometry to transform complex analyses into an efficient workflow. The interface enables users to select five crystal systems (cubic, tetragonal, hexagonal, orthorhombic, monoclinic), input X-ray diffraction angles (2θ) and Miller indices (hkl), and automatically compute lattice parameters. Three-dimensional visualizations enhance interpretability of results, while open-source accessibility ensures broad applicability. Validated against reference data, the tool achieves errors ranging from 0.03% to 2.88%. By bridging advanced material characterization with sustainable development goals, this GUI democratizes crystallographic analysis for interdisciplinary teams, empowering researchers in energy harvesting, catalysis, and eco-friendly material design. Its computational efficiency and user-centric design support transdisciplinary innovation, reinforcing the role of accessible tools in accelerating sustainable technologies. **Keywords:** Crystal lattice parameter, X-ray diffraction, Cramer-cohen algorithm, GUI

1 Introduction

Accurate characterization of crystalline materials is critical for advancing technologies that enhance ecosystem resilience, such as low-carbon energy systems, pollution remediation frameworks, and sustainable infrastructure—applications where structural precision directly impacts environmental and economic sustainability [1,2]. X-ray diffraction (XRD) serves as a cornerstone technique for this purpose, enabling researchers to derive crystal structures and lattice parameters via Bragg's Law [3]. However, traditional XRD data analysis remains labor-intensive, particularly when dealing with the seven crystal systems: cubic, tetragonal, orthorhombic, hexagonal, rhombohedral, monoclinic, and triclinic. Each system requires unique equations to calculate interplanar spacing due to differences in lattice symmetry [4]. Previous studies have focused predominantly on cubic, tetragonal, and hexagonal systems, as these structures are more common and exhibit lower computational complexity [5]. In

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contrast, low-symmetry systems (e.g., monoclinic) have received less attention due to their mathematical challenges and their perceived rarity in conventional applications, despite their growing relevance in sustainable materials (e.g., metal-organic frameworks for carbon capture) [6].

The Cramer-Cohen method, a determinant-based approach for solving linear matrix equations, provides a foundational framework for lattice parameter analysis [7]. When integrated with modern computational tools like Python—a language widely adopted for its scientific libraries (e.g., NumPy for matrix operations)—this method enables efficient analysis of diverse crystal systems [8]. To improve accessibility, an intuitive Graphical User Interface (GUI) reduces the technical barrier to performing complex calculations, aligning with human-computer interaction principles that prioritize usability in specialized workflows [9]. Historically, crystallography software tools were limited in scope, often supporting only high-symmetry systems (e.g., Cubic or Hexagonal), which restricted their utility for emerging materials with low-symmetry lattices [10]. Recent advancements in materials science, particularly the demand for sustainable technologies (e.g., perovskite solar cells, solid-state batteries), have underscored the need for precise and adaptable lattice parameter analysis tools capable of handling structurally diverse systems [11].

To address these gaps, we: 1) developed a lightweight, Python-based application with a GUI to streamline lattice parameter calculations via the Cramer-Cohen method; 2) assessed the accuracy of the application across five crystal systems (cubic, tetragonal, hexagonal, orthorhombic, and monoclinic); 3) visualized the crystal systems; and 4) compared the tool's performance and features against existing crystallography software.

2 Method

A Python-based program was developed that leverages the Cramer-Cohen method as its core algorithm for computing lattice parameters from X-ray diffraction (XRD) data. The program integrates Bragg's Law to calculate distance between parallel layers of atoms (interplanar spacing) in a crystal. The performance of the program was evaluated by testing its ability to accurately compute lattice parameters across various crystal systems, including cubic, tetragonal, hexagonal, orthorhombic, and monoclinic structures. Accuracy was benchmarked against established reference data to ensure reliability.

2.1 Mathematical foundations and computational workflow

2.1.1 Bragg's Law

Braggs's Law governs the relationship between X-ray wavelength, diffraction angle, and interplanar spacing, where $h, k, and\ l$ are Miller indices of the crystallographic plane [3]. For a crystal system with lattice parameters $(a, b, c, \alpha, \beta, and\ \gamma)$, d_{hkl} is determined by the metric tensor of the unit cell. For example, in a cubic system ($a = b = c, \alpha = \beta = \gamma = 90°$) [12], the interplanar spacing (d) simplifies to equation (1):

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \tag{1}$$

For lower-symmetry systems (e.g., monoclinic), , d_{hkl} requires solving a system of equation derived from the crystal's unique metric tensor. For a detailed derivation of each crystal system, see Cullity & Stock [3].

2.1.1 Cramer-Cohen Method

The Cramer-Cohen method solved system of linear equations arising from Bragg's Law to calculate lattice parameters. This transformed the system into a matrix equation ($\mathbf{Ax} = \mathbf{B}$), where **x** contains terms proportional to $1/a^2$, $1/b^2$, *and* $1/c^2$. The matrix **A** (constructed from Miller indices h, k, l) and vector **B** (derived from $\sin^2\theta$ values) were solved using Cramer's rule [15], for example, the lattice parameters of the orthorhombic crystals are characterized by $a \neq b \neq c$ and $\alpha = \beta = \gamma = 90°$ [12]. According to Cullity & Stock [3], the interplanar spacing (d) is given by equation (2):

$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \tag{2}$$

Substituting equation (2) into Bragg's law ($2d_{hkl}\sin\theta = n\lambda$) [13] and following Cohen's derivation ($D\sin^2 2\theta$) [5], the formula transforms into equation (3):

$$\sin^2\theta = U_\phi + V_\chi + W_\psi + T\zeta \tag{3}$$

Where $U = \frac{\lambda^2}{4a^2}$, $V = \frac{\lambda^2}{4b^2}$, $W = \frac{\lambda^2}{4c^2}$, $T = \frac{D}{10}$, $\phi = h^2, \chi = k^2$, $\psi = l^2, and\ \zeta = 10\sin^2 2\theta$. Then, equation (3) was transformed into a linear matrix shown in equation (4):

$$\begin{bmatrix} \sum\phi^2 & \sum\phi\chi & \sum\phi\psi & \sum\phi\zeta \\ \sum\phi\chi & \sum\chi^2 & \sum\chi\psi & \sum\chi\zeta \\ \sum\phi\psi & \sum\chi\psi & \sum\psi^2 & \sum\psi\zeta \\ \sum\phi\zeta & \sum\chi\zeta & \sum\psi\zeta & \sum\zeta^2 \end{bmatrix} \begin{bmatrix} U \\ V \\ W \\ T \end{bmatrix} = \begin{bmatrix} \sum(\phi\sin^2\theta) \\ \sum(\chi\sin^2\theta) \\ \sum(\psi\sin^2\theta) \\ \sum(\zeta\sin^2\theta) \end{bmatrix} \tag{4}$$

The matrix above solved using the Cramer's rule [14]. For a detailed matrix derivation of each crystal s, see Suryanarayana [5].

2.2 GUI's algorithm

The program employs the Cramer-Cohen method as its core algorithm to compute lattice parameters, with a graphical user interface (GUI) developed using the wxPython library. Upon execution, users interact with the GUI to select the crystal systems by entering a numerical code, specify the number of X-ray diffraction data rows, and input diffraction angles (2θ) and corresponding Miller indices (hkl) sequentially. This numerical implementation, developed in Python using the NumPy library for matrix operations, outputs the refined lattice parameters and generates a D visualization of the Miller indices within the wxPython GUI framework (Figure 1).

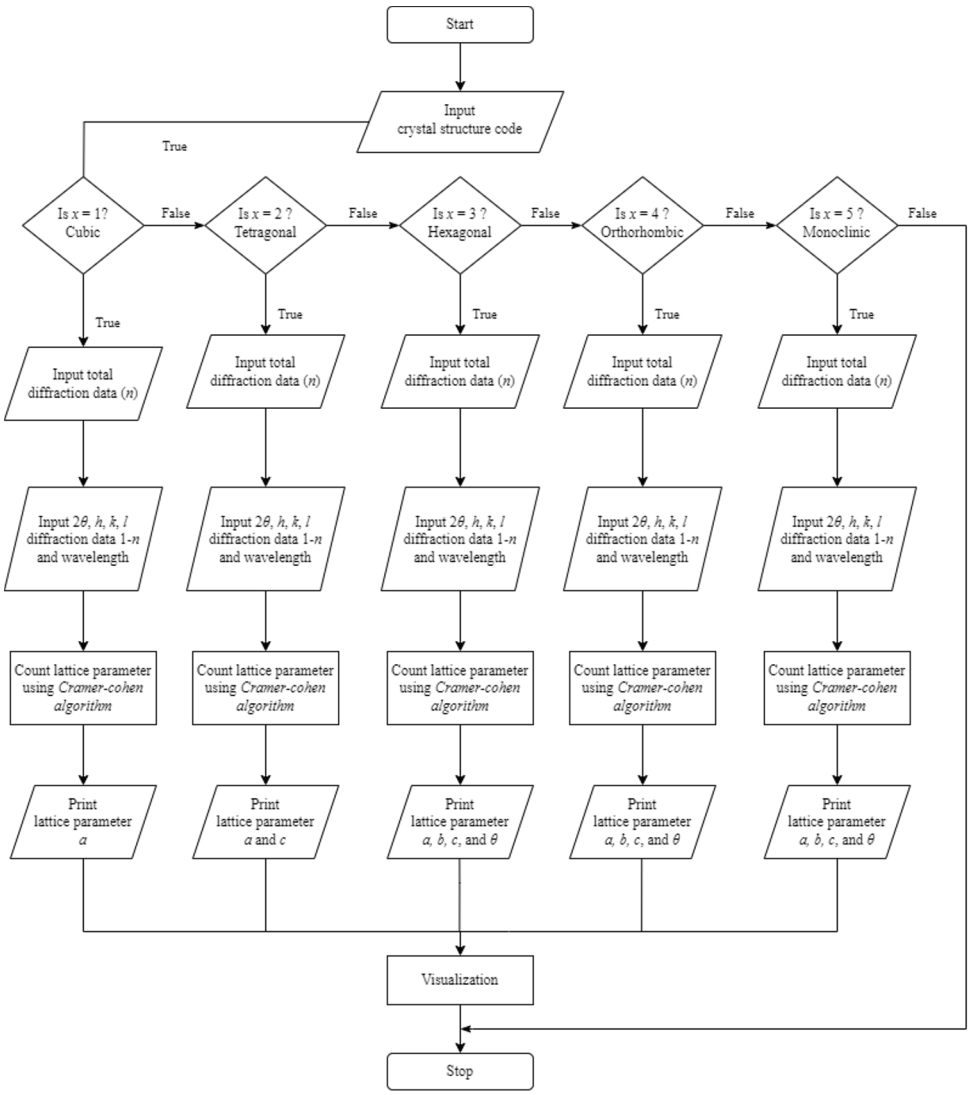

Fig. 1. Representation of the process by which the program calculates lattice parameters based on user inputs.

2.3 Accuracy assessment

The program's accuracy was evaluated using reference data from the International Centre for Diffraction Data (ICDD) across five crystal systems (cubic, tetragonal, hexagonal, orthorhombic, and monoclinic). Accuracy assessment is carried out by comparing the calculation results against reference data, using the error value as an indicator of algorithm resolution [15]. The error value is calculated using equation (5).

$$Error\ value\ (\%) = \left(\frac{|Calculated\ value\ -\ Reference\ value\ |}{Reference\ value}\right) \times 100 \qquad (5)$$

3 Results and Discussions

3.1 GUI development

The GUI program was developed in Python using the wxPython framework, integrating the Cramer-Cohen method for calculations and Matplotlib for real-time visualization of Miller indices. The interface guides users through an intuitive workflow: first, selecting the crystal system via a numerical code (1: cubic, 2: tetragonal, 3: hexagonal, 4: orthorhombic, 5: monoclinic); second, inputting diffraction angles (2θ) and corresponding Miller indices (hkl) into dedicated fields. The GUI then displays the calculated lattice parameters and options to visualize the crystal systems (Figure 2). The GUI's design eliminates command-line dependencies, enabling non-experts such as chemists or materials engineers to perform complex crystallographic analyses—critical for collaborative development of sustainable technologies like perovskite solar cells or solid-state battery materials [11].

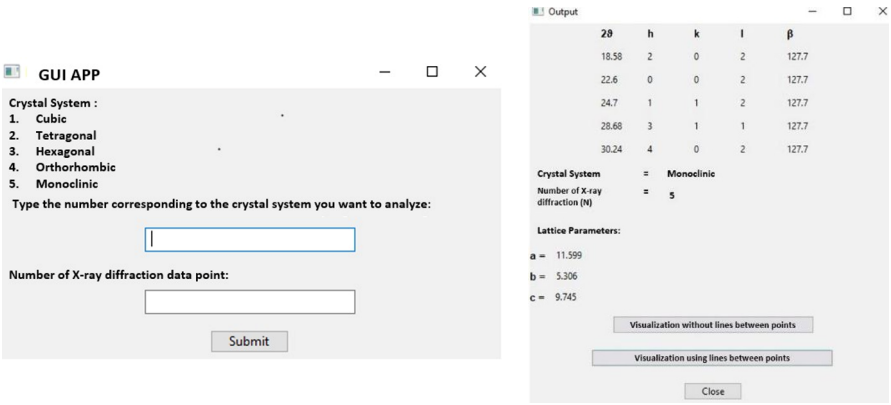

Fig. 2. Main page of the GUI for selecting crystal systems (left) and lattice parameter calculation results (right).

3.2 Accuracy assessment of lattice parameter calculations

The program's accuracy was validated against reference data from the International Centre for Diffraction Data (ICDD) across five crystal systems, with percentage errors ranged from 0.03% to 2.88% (Figure 3 and Table 2). Performance testing showed high accuracy, particularly for cubic and orthorhombic systems, with average errors of 0.20% and 0.30%, respectively. In the cubic system, results for NaCl (0.30%) and β-Ag_3In (0.09%) demonstrated precision. The hexagonal system showed moderate accuracy, as seen in GaN (0.09%) and NiS (0.93%). GaN used in energy-efficient power electronics, electric vehicles, and LED lighting [16]. The tetragonal system showed accurate results for TiO_2 (0.026% for a and b, 0.021% for c) but higher errors for $Pb(ZrO_2Ti_{0.48})O_3$. TiO_2 used in key material in dye-sensitized solar cells and perovskite solar cells [17]. Monoclinic systems showed errors ranging from 0.25% to 1.77%. These results underscore the tool's utility in advancing materials for renewable energy systems, where precise lattice parameters dictate device efficiency [18].

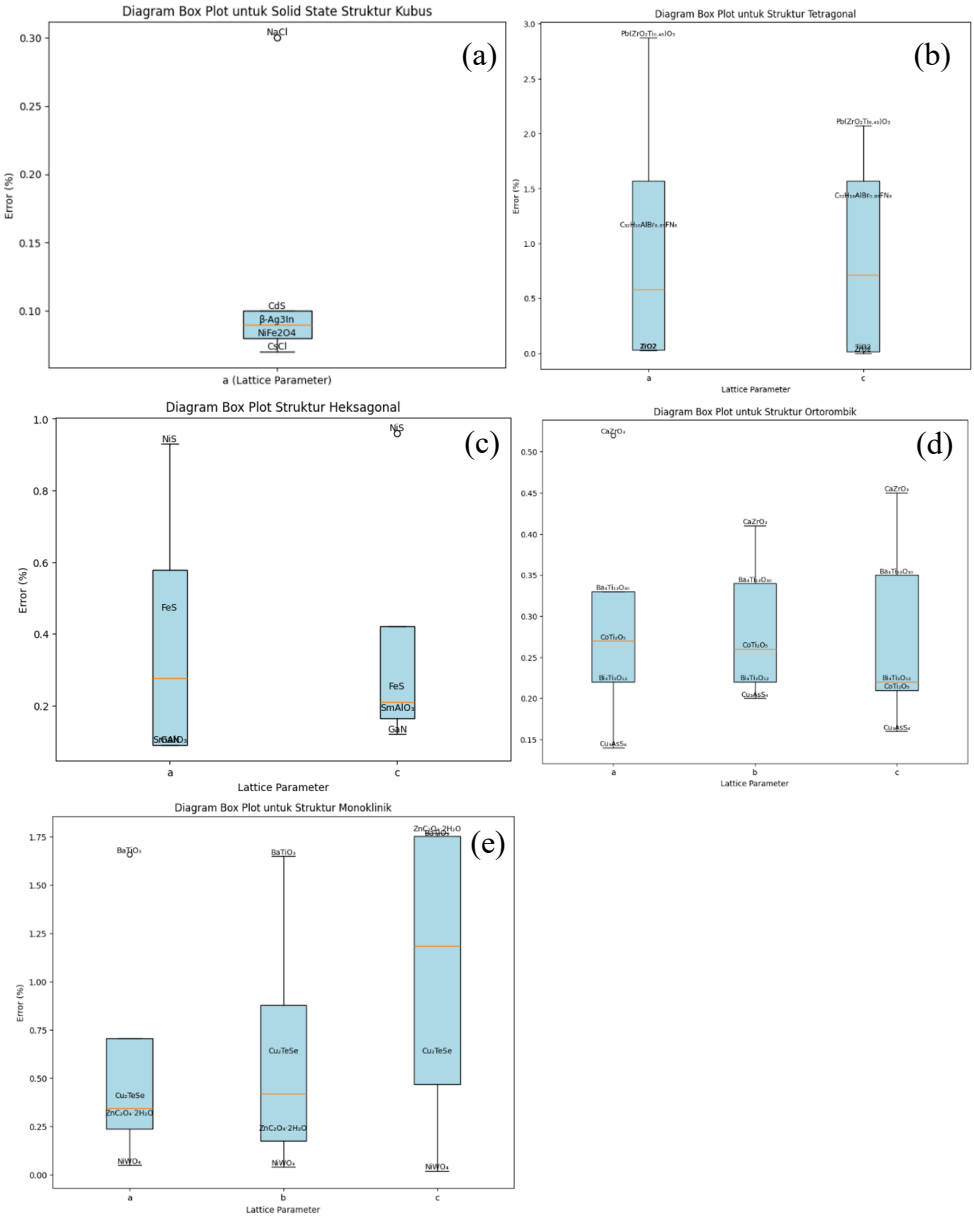

Fig. 3. Boxplot showing the error values for cubic (a), tetragonal (b), hexagonal (c), orthorhombic (d), and monoclinic (e) systems.

Table 2. Error value of calculated lattice parameters for five crystal systems.

Crystal systems	Material sample	Error value of lattice parameters (%)		
		a	***b***	***c***
Cubic	NaCl	0.30	0.30	0.30
	β-Ag3In	0.09	0.09	0.09
	CdS	0.10	0.10	0.10
	CsCl	0.07	0.07	0.07
	NiFe2O4	0.08	0.08	0.08
Tetragonal	Ti02	0.026	0.026	0.021
	$C_{32}H_{16}AlBr_{0.89}FN_8$	1.134	1.134	1.403
	ZrO2	0.028	0.028	0.000
	$Pb(ZrO_2Ti_{0.48})O_3$	2.874	2.874	2.074
Hexagonal	FeS	0.46	0.46	0.24
	NiS	0.93	0.93	0.96
	GaN	0.09	0.09	0.12
	$SmAlO_3$	0.09	0.09	0.18
Orthorhombic	$CaZrO_3$	0.52	0.41	0.45
	$Bi_4Ti_3O_{12}$	0.22	0.22	0.22
	Cu_3AsS_4	0.14	0.20	0.12
	$Ba_4Ti_{13}O_{30}$	0.33	0.34	0.35
Monoclinic	$NiWO_4$	0.05	0.04	0.02
	Cu_2TeSe	0.39	0.62	0.62
	Cu_3AsS_4	0.14	0.20	0.12
	$BaTiO_3$	1.66	1.65	1.75
	$ZnC_2O_4 \cdot 2H_2O$	0.30	0.22	1.77

3.3 Crystal systems visualization

The Matplotlib-integrated visualization module maps Miller indices (hkl) into 3D representations of crystallographic planes, enabling users to correlate diffraction patterns with atomic arrangements (Figure 4 and Figure 5). This visual feedback bridges the gap between theoretical diffraction data and practical material design.

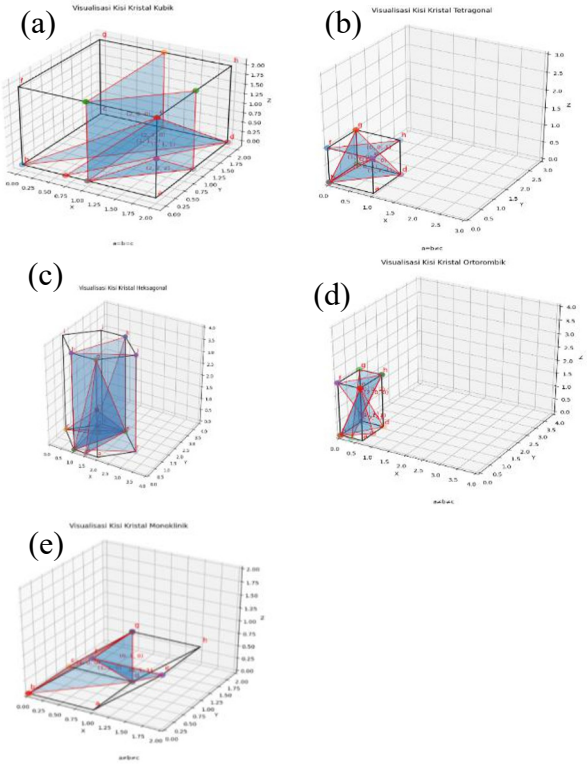

Fig. 4. Visualization of Miller indices for (a) cubic, (b) tetragonal, (c) hexagonal, (d) orthorhombic, and (e) monoclinic crystal systems.

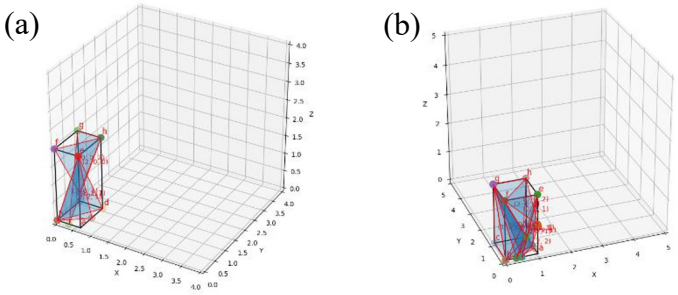

Fig. 5. Visualization of orthorhombic systems for (a) $CaZrO_3$ and (b) Cu_3AsS_4.

3.4 GUI usability and comparative functionality

The GUI was benchmarked against established tools (Vesta, Diamond, Mercury) in functionality, cost, and accessibility (Table 2). Unlike proprietary software requiring licenses, this open-source tool eliminates financial barriers, democratizing access for academic and low-resource industrial labs. Its simplified workflow reduces the learning curve for non-physicists, such as environmental engineers analyzing catalyst structures or educators teaching crystallography. While specialized tools like Vesta offer advanced symmetry analysis, this program offer calculation for low-symmetry systems (e.g., monoclinic).

Table 2. Comparison of features in the developed GUI application and other related applications.

Features and Description of the GUI Application	Developed GUI app	Vesta	Diamond	Mercury
Can the application calculate lattice parameters from XRD data?	V			
Does the application provide crystal systems visualization?	V	V		
Is the application free to use?	V	V		
Can visualization results be exported?	V	V	V	
Does the application allow selecting different crystal systems?	V	V		V
Is the application user-friendly, especially for beginners?	V	V		
Is the application supported on multiple platforms (Windows, macOS, Linux)?	V	V		

4 Conclusion

To bridge existing gaps in accessible and user-friendly crystallographic tools, this study introduces a lightweight, Python-based application with an intuitive wxPython graphical interface for lattice parameter determination via the Cramer-Cohen method. The tool's performance was rigorously validated across five crystal systems (cubic, tetragonal, hexagonal, orthorhombic, and monoclinic), demonstrating accuracy ranged from 0.03% to 2.88% of reference values. Integrated 3D visualization capabilities enable direct rendering of Miller indices and crystal systems, enhancing interpretability of diffraction patterns. Comparative benchmarking against established software (Vesta, Diamond, Mercury) highlights this tool's advantages in computational efficiency, open-source accessibility, and reduced dependency on proprietary frameworks—critical for educational and resource-limited settings.

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