


Crystal Lattice: An alternative software for calculating lattice parameters from X-ray diffraction data


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Abstract: In materials synthesis research, understanding the lattice parameters is crucial for determining the phase and evolution of a material's microstructure. Crystal Lattice is user-friendly, free software designed to calculate the lattice parameters of the seven crystalline systems using one or more X-ray diffraction (XRD) planes. Developed in an accessible programming environment like Visual Studio, this program employs analytical methods to calculate the lattice parameters. To use the software, users need to input the diffraction angle (2θ) and the Miller indices (hkl); with this information, the program determines the lattice parameters. Additionally, Crystal Lattice can calculate the crystallite size based on the diffraction angle (2θ) and the full width at half maximum (FWHM). The software validation used information from the ICSD (Inorganic Crystal Structure Database) crystallographic card of different chemical compounds. The data was processed using the equation corresponding to each crystal structure. The results were compared with the information provided in the ICSD crystallographic card data, obtaining a mean error of 0.059%.

Keywords: X-ray diffraction; lattice parameters; Miller indices; crystal structure; software.

Resumen: En la investigación de síntesis de materiales, comprender los parámetros de red es crucial para determinar la fase y la evolución de la microestructura de un material. Crystal Lattice es un software gratuito e intuitivo diseñado para calcular los parámetros de red de siete sistemas cristalinos mediante uno o más planos de difracción de rayos X (DRX). Desarrollado en un entorno de programación accesible como Visual Studio, este programa emplea métodos analíticos para calcular los parámetros de red. Para utilizar el software, los usuarios deben introducir el ángulo de difracción (2θ) y los índices de Miller (hkl); con esta información, el programa determina los parámetros de red. Además, Crystal Lattice puede calcular el tamaño de los cristallitos basándose en el ángulo de difracción (2θ) y el ancho total a la mitad del máximo (FWHM, por sus siglas en inglés). Para la validación del software, se utilizó información de la carta cristalográfica de la base de datos de estructuras cristalinas inorgánicas (ICSD, por sus siglas en inglés) de diferentes compuestos químicos. Los datos se procesaron utilizando la ecuación correspondiente a cada estructura cristalina. Los resultados se compararon con la información proporcionada en los datos de la carta cristalográfica ICSD, obteniendo un error medio de 0.059%.

Palabras clave: Difracción de rayos X; parámetros de red; índices de Miller; estructura cristalina; software.

Introduction

A crucial step for researching crystal structure, phase identification, solubility range, and physical characteristics is the estimation of lattice constants from

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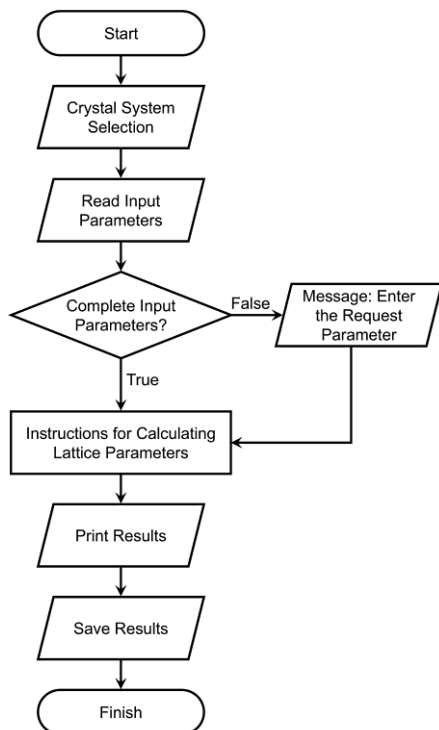
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X-ray diffraction (XRD) data (Nikam, 2021; Oponowicz et al., 2020), and calculations that previously had to be solved by hand can now be performed using software. Although most people use spreadsheets to analyze lattice parameters, applications have also been developed to analyze lattice parameters, such as one created on Android by Kurniawan et al. (Kurniawan & Irzaman, 2021). While there are commercial programs available to determine lattice parameters, many of these require a paid license and limit the functionality of their trial versions. Hence, as another alternative to calculate the lattice parameters, a software program called "Crystal Lattice" was developed using the Visual Studio programming language. The algorithm is based on the known Bragg's law, the Scherrer equation, and the equations of the seven crystalline systems (Cullity & Stock, 2014). Therefore, the software presented in this paper is aimed at determining the crystallographic parameters by incorporating some key considerations: simplifying the calculation and employing a uniform methodology. In addition, information from ICSD crystallographic cards of F_3O_4 (cubic), SiO_2 (hexagonal), ZrO_2 (tetragonal), Sb_2Se_3 (orthorhombic), B_4C (rhombohedral), Lu_2O_5Si (monoclinic), and $Fe_3^{+2}Al_4(PO_4)_4(OH)_6 \cdot 2H_2O$ (triclinic) were used to determine the lattice parameters and validate the software.

Code description

The software is designed to select any of the seven crystal systems from a menu and enter the requested parameters. Fig. 1 provides an overview of the flowchart for calculating lattice parameters.

Fig. 1. Flow chart for calculating lattice parameters.



The process starts when the user selects the crystalline system, then the information is entered, such as the wavelength with which the XRD analysis was carried out, the form factor, the angles where the reflection occurs, FWHM, the Miller indices (hkl), and angles of the crystal structure. Finally, the results obtained can be saved in a .xlsx file.

Methodology

The script was developed in Visual Studio version 2022. To validate the "Crystal Lattice" software, the lattice parameters of quartz (SiO_2) which has a hexagonal structure were calculated, and the results obtained were compared with the reference (Proffen et al., 2005). The values for SiO_2 are $a = 4.914 \text{ \AA}$ and $c = 5.407 \text{ \AA}$ according to ICSD card No. 98-015-4289. The crystallite size (D) was determined using the Scherrer equation (1) (Cullity & Stock, 2014):

$$D = \frac{K\lambda}{\beta \cos \theta} \quad (1)$$

where K is the form factor, λ is the wavelength of CuK_α radiation (1.5406 \AA), β is FWHM of the X-ray diffraction peak, and θ is the Bragg's angle ($^\circ$). Equations (2) and (3) were used to determine the structural parameters, such as the lattice constant (a) and interplanar spacing (d_{hkl}) [11]:

$$d_{hkl} = \frac{\lambda}{2 \sin \theta} \quad (2)$$

and,

$$\frac{1}{d_{hkl}^2} = \frac{4}{3} \left(\frac{h^2 + hk + k^2}{a^2} \right) + \frac{l^2}{c^2} \quad (3)$$

The FWHM was obtained by performing a fit with a Gaussian function in Origin software version 2021 to input this data and calculate the crystallite size. In addition, the following equations from Table 1 were used and programmed into the source code to test the crystal structures of F_3O_4 (cubic), Lu_2O_5Si (monoclinic), Sb_2Se_3 (orthorhombic), B_4C (rhombohedral), ZrO_2 (tetragonal), and $Fe_3^{+2}Al_4(PO_4)_4(OH)_6 \cdot 2H_2O$ (triclinic) and determine the lattice parameters.

Table 1. Equations to determine lattice parameters a , b , and c .

Crystalline System	Equations
Cubic	$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$
Tetragonal	$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$
Rhombohedral	$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2)\sin^2 \alpha + 2(hk + kl + hl)\cos^2 \alpha - \cos \alpha}{a^2(1 - 3\cos^2 \alpha + 2\cos^3 \alpha)}$
Orthorhombic	$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$
Monoclinic	$\frac{1}{d^2} = \frac{1}{\sin^2 \beta} \left(\frac{h^2}{a^2} + \frac{k^2 \sin^2 \beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl \cos \beta}{ac} \right)$
Triclinic	$\frac{1}{d^2} = \frac{\left(\frac{h^2}{a^2} \sin^2 \alpha + \frac{k^2}{b^2} \sin^2 \beta + \frac{l^2}{c^2} \sin^2 \gamma + \frac{2kl}{bc} (\cos \beta \cos \gamma - \cos \alpha) + \frac{2hl}{ac} (\cos \alpha \cos \gamma - \cos \beta) + \frac{2hk}{ab} (\cos \alpha \cos \beta - \cos \gamma) \right)}{1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma}$

Results

Fig. 2 shows the X-ray diffraction pattern of quartz. All diffraction peaks were indexed and corresponded to a hexagonal structure according to ICSD card No. 98-015-4289. To determine the crystallite size, some planes were selected to perform a fit with a Gaussian function and obtain the FWHM data for each selected diffraction peak as listed in Table 2. The planes chosen for the hexagonal structure must be of the types (XX0) and (00X). If other types of planes are selected, the software will not correctly determine the lattice parameters, as the variables will become indeterminate.

Fig. 2. X-ray diffraction patterns of quartz.

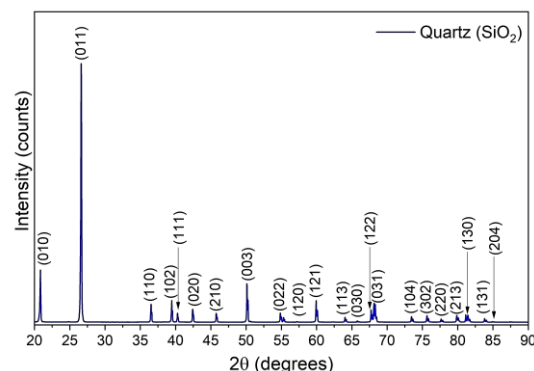


Table 2. Fitting parameters calculated with the Gaussian function of quartz.

hkl	y ₀	x _c	Area	FWHM	R ²	D (nm)	d (Å)
010	0.0117	20.83965	0.02481	0.12834	0.96834	62.9	4.25911
110	0.00161	36.54217	0.01017	0.16124	0.95472	51.9	2.45699
020	0.00302	42.43275	0.00497	0.10096	0.99443	84.4	2.12854
003	0.00193	50.60098	0.00015	0.07307	0.96029	120.3	1.80244
120	0.00069	57.21511	0.00015	0.09189	0.95063	98.5	1.60879
030	0.00079	65.77100	0.00039	0.09435	0.98764	100.3	1.41870
220	0.00152	77.64942	0.00125	0.10838	0.99318	94.1	1.22867
130	0.00381	81.44084	0.00367	0.14304	0.99384	73.3	1.18077
Average						85.7	

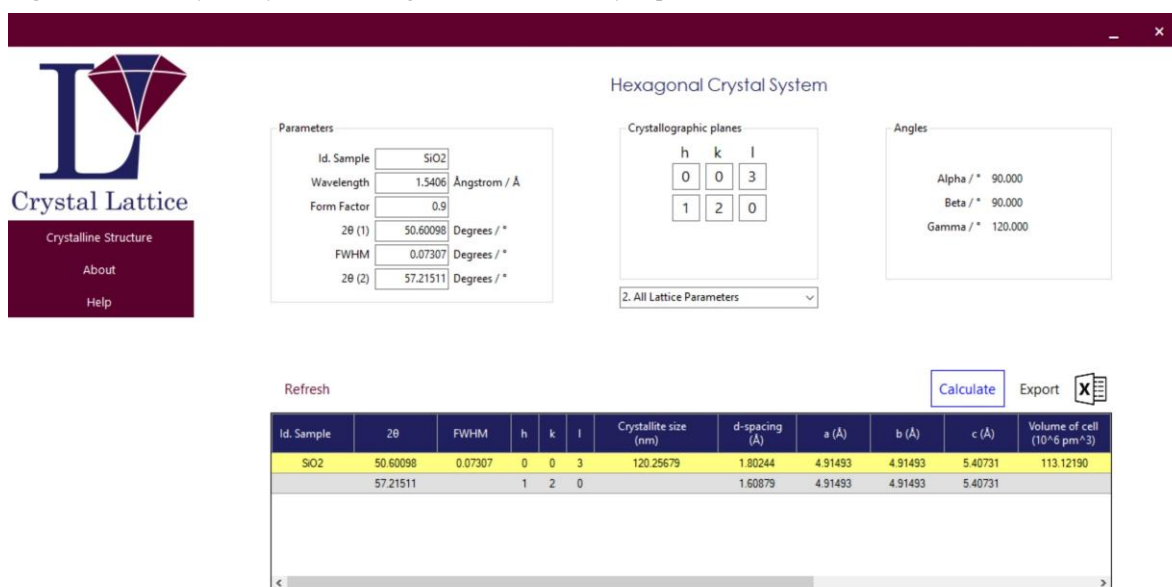
The results of the lattice parameters of quartz are listed in Table 3. The data obtained with the software were compared with the information in reference ICSD 98-015-4289. As a result, a mean error of 0.059% was

obtained. Fig. 3 shows a screenshot of the software in the hexagonal crystal system determining the lattice parameters.

Table 3. Lattice parameters of quartz.

Lattice Parameter (Å)								
<i>a</i>					<i>c</i>			
hkl	Software Reference	Software Experimental	Literature	% Error	Software Reference	Software Experimental	Literature	% Error
010	4.91395	4.91799		0.082				
110	4.90196	4.91399		0.245				
020	4.91397	4.91566		0.034				
003	4.91401	4.91493	4.914	0.019	5.40701	5.40731	5.407	0.006
120	4.91339	4.91493		0.031				
030	4.91399	4.91452		0.011				
220	4.91400	4.91467		0.014				
130	4.91400	4.91596		0.040				
Average	4.91241	4.91533		0.059				

Fig. 3. Screenshot of the software showing the results obtained for quartz.



Notably, the results calculated through the software exhibit minimal variation across different sets of planes. This indicates that it is feasible to determine the lattice parameters for the hexagonal structure using only two diffraction planes. Table 4 shows the results for F₃O₄

(cubic), ZrO₂ (tetragonal), B₄C (rhombohedral), Sb₂Se₃ (orthorhombic), Lu₂O₅Si (monoclinic), and Fe₃⁺²Al₄(PO₄)₄(OH)₆·2H₂O (triclinic) specimens that were used to test the remaining crystal systems. However, to calculate the lattice parameters, certain

crystallographic planes must be chosen because the program is based on the equations for calculating the d-spacing in which some Miller indices must be equal to zero. The results obtained indicate that the developed software is suitable for all seven crystalline systems since

the number of unknown lattice parameters matches the minimum number of diffraction planes necessary, which demonstrates that the software provides reasonably accurate calculations.

Table 4. Lattice parameter values of several specimens using Crystal Lattice software and ICSD cards as reference.

Specimen	hkl	d (Å)	a (Å)	b (Å)	c (Å)	
F ₃ O ₄ 01-079-0418	311	2.53222	8.39842			Crystal Lattice (Fleet, 1986)
		2.53224	8.39850			
ZrO ₂ 01-089-6976	002	2.63504	3.64004		5.27007	Crystal Lattice
	110	2.57390				
	002	2.63500	3.64000		5.27000	(Sham et al., 1998)
	110	2.57387				
B ₄ C 00-035-0798	003	4.03304	5.60629		12.09911	Crystal Lattice
	110	2.80315				
	003	4.03303	5.60030		12.0860	(Clark & Hoard, 1943)
	110	2.80314				
Sb ₂ Se ₃ 00-015-0861	040	2.94496				Crystal Lattice
	430	2.33702	11.63279	11.77982	3.98312	
	061	1.76100				
	040	2.94500				(Swanson et al., 1964)
	430	2.33700	11.63300	11.78000	3.98500	
	061	1.76100				
Lu ₂ O ₅ Si 98-008-9624	110	5.31417				Crystal Lattice
	200	4.35666	8.98714	6.70571	6.59500	
	102	2.78859				
	110	5.31429				(Müller-Bunz & Schleid, 1999)
	200	4.35659	8.98700	6.70600	6.59500	
	102	2.78858				
Fe ³⁺ ₂ Al ₄ (PO ₄) ₄ (OH) ₆ ·2H ₂ O 00-036-0403	300	3.87802				Crystal Lattice
	330	1.55789	11.78548	5.11566	13.59241	
	029	1.28020				
	300	3.87800				(Sturman et al., 1981)
	330	1.55790	11.78900	5.11700	13.59000	
	029	1.28020				

Conclusions

The Crystal Lattice software was developed using a simple programming language and features an easy-to-use interface for end users. This program enables users to calculate lattice parameters from data obtained from X-ray diffraction patterns. Its validation performance shows that it can accurately determine lattice parameters for structures ranging from simple cubic to complex triclinic structures. Additionally, Crystal Lattice supports

the use of both high and low angle diffraction planes for lattice parameter calculations. The program showed a small mean error of 0.059%, indicating a very low probability of error in its calculations. Crystal Lattice is well-suited for the routine analysis of variations in lattice parameters of materials and is accessible to both students and scientists.

Software availability

Reyes-Valdez, J.J., Benito-Santiago, S.E. & Espíndola-Flores, A.C. Crystal Lattice Version 1.0 [Software]. 20-04-2024.

Download link:

https://drive.google.com/uc?export=download&id=1ckhZxn_BD_buLPZkK2zJUfO5RwMNqQW

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