Python-based Program for Analysing Lattice Parameter of Cubic and Tetragonal Crystal Structure

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Abstract. A program for analysing lattice parameter of a crystal structure has been successfully created based on Python programming language using the Google Collaboratory service, so it can be accessed through a PC or smartphone as long as internet access is available. This program can be used to calculate lattice parameter of a crystal structure with x-ray diffraction data as the input. Crystal structures that can be calculated for its lattice parameter are cubic and tetragonal. The program will ask for the type of crystal structure of the data, along with diffraction angles and miller indices. The input will be processed using the Cramer-Cohen method according to the previously entered crystal structure. By also entering the wavelength used, the output of this program is the lattice parameter in the angstrom unit. The percentage of error of this program’s output is extremely low.

1. Introduction
Solid substances are often found in various areas of human daily life. Utilization of solids is carried out by analysing the characteristics of these solids. Various characteristics of the solid material can be determined by analysing the structure and phase of the crystal, also its lattice parameter [1]. Research on analysing the crystal structure of a solid material is very interesting, as did previous researchers. Previous researchers have succeeded in analysing and determining the crystal structure of various materials, including lithium aluminum silicate glass-ceramics [2] and selenium-doped hydroxyapatite [3].

One of the common experimental methods used in determining the structure, phase and lattice parameter of a crystal is x-ray diffraction (XRD). X-ray diffraction uses the phase difference that occurs between x-rays hitting the parallel lattice planes to calculate the crystal lattice parameter based on Bragg’s Law [4]. The output resulting from x-ray diffraction is a graph imaging the relationship between the diffraction angle for each miller index and the intensity of the x-rays received back by the detector.

There are seven types of crystal structures, i.e. Cube, Tetragonal, Orthorhombic, Hexagonal, Rhombohedral, Monoclinic and Triclinic [5]. Each structure has a different equation for distance between parallel lattice planes (d-spacing). The simplest method of lattice parameter’s analysis is the Cramer-Cohen method. The Cramer method is a method to solve linear matrix equations by counting the determinant of the matrix involved in the equation [6].

Over time, mathematical equations that previously had to be solved by hand can be done using applications or programs. One programming language that has been widely used to solve mathematical equations is Python. Research on the Python programming language is very interesting, as did previous researchers. Previous researchers have successfully applied the python programming language to simplify various types of mathematical and physical cases, including Python to learn programming [7], PDB File Parser and Structure Class Implemented in Python [8], Emcee V3: A
Python Ensemble Sampling Toolkit for Affine-Invariant MCMC [9], pyhf: Pure-python Implementation of HistFactory Statistical Models [10].

Most people use Microsoft Excel to analyse lattice parameter. Research on making application to analysing lattice parameter has been carried out previously as an android-based application [11]. Apart from using the application, lattice parameter analysis can also be done with code-based program using Python as the programming language. This research was conducted with the aim of providing an analysis tool for crystal structure lattice parameter that is easier and more efficient to use without additional occupied memory on the device and can be accessed anywhere as long as the internet service is provided.

2. Method
The first step taken in this research is the literature review. The next step is building the code-based program with Cramer-Cohen method as an algorithm and Python as the programming language. The final step in this research is testing the performance of the program in performing calculations.

2.1. Literature Review
The literature review is the first step taken in this research. Topics that being reviewed from the literature are about Bragg’s law, its applications for XRD, crystal structure and Cramer-Cohen method for analysing lattice parameter in cubic and tetragonal crystal structure.

2.1.1. Bragg’s law.
Bragg's law is the main principle used in the x-ray diffraction method. Two x-rays hitting some parallel lattice planes must interfere each other. Constructive interference happens when the difference path length of two rays is equal to multiple of positive integers of the x-ray wavelength used. Bragg's law is mathematically formulated in equation (1),

$$2d \sin \theta = n\lambda$$

which $d$ represents path’s length between two lattice planes with same $hkl$ value [12]. For analysing two rays in two neighboured parallel planes, substitute $n = 1$, so equation (2) is obtained.

$$\frac{1}{d} = \frac{2\sin \theta}{\lambda}$$

2.1.2. Lattice parameter.
Those seven types of crystal structure has their unique characteristic of lattice parameter compare to the others [5]. Lattice parameter is important to be determined, because it describes the size of the unit cell of a material. This knowledge could lead to many different potential applications of the material [13]. Lattice parameter contains a set of constants denoted as “a”, “b”, “c”, “α”, “β” and “γ”. “a”, “b” and “c” describe distance between atoms on unit cell’s x, y and z axis, respectively. Meanwhile, “α”, “β” and “γ” describe angle between unit cells’s y and z axis, x and z axis, also x and y axis, respectively.

2.1.3. Cramer-Cohen method for cubic crystal structure.
A cube crystal structure that has unit cells with the lattice parameter $a = b = c$ and $\alpha = \beta = \gamma = 90^\circ$ [5]. Therefore, a cube crystal needs 1 lattice parameter only to describe its characteristics, which is usually denoted as 'a'. The d-spacing in the cube crystal is shown in equation (3),

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$
with $h$, $k$ and $l$ are plane’s dimensions on $x$, $y$ and $z$ axis, respectively [14]. Equation (3) is then compared with equation (2), so equation (4) is obtained.

$$\frac{h^2+k^2+l^2}{a^2} = \frac{4\sin^2 \theta}{\lambda^2}$$  \hspace{1cm} (4)

$$\sin^2 \theta - \frac{\lambda^2}{4a^2} (h^2+k^2+l^2) = 0$$  \hspace{1cm} (5)

By replacing zero in the equation above with error during measurement, according to what Cohen has derived, that is expressed as $D \sin^2 2\theta$ [15], equation (6) is obtained,

$$\sin^2 \theta - \frac{\lambda^2}{4a^2} (h^2+k^2+l^2) = D \sin^2 2\theta$$  \hspace{1cm} (6)

$$\sin^2 \theta - \frac{\lambda^2}{4a^2} (h^2+k^2+l^2) + D \sin^2 2\theta$$  \hspace{1cm} (7)

$$\sin^2 \theta = S \chi + T \psi$$  \hspace{1cm} (8)

with $S = \frac{\lambda^2}{4a^2}$, $T = \frac{D}{10}$, $\chi = h^2+k^2+l^2$ and $\psi = 10\sin^2 2\theta$. Transform equation (8) into a linear matrix equation shown in equation (9).

$$\begin{pmatrix} \sum \chi \sin^2 \theta \\ \sum \psi \sin^2 \theta \end{pmatrix} = \begin{pmatrix} \sum \chi^2 \\ \sum \psi \chi \\ \sum \psi^2 \end{pmatrix} \begin{pmatrix} S \\ T \end{pmatrix}$$  \hspace{1cm} (9)

Solution of the equation above can be found using the Cramer method. This is Cramer-Cohen method for cubic crystal structure [11].

2.1.4. Cramer-Cohen method for tetragonal crystal structure.

A tetragonal crystal structure is a crystal structure that has unit cells with the lattice parameter $a = b \neq c$, but $\alpha = \beta = \gamma = 90^\circ$ [5]. Therefore, a tetragonal crystal need 2 lattice parameters describe its characteristics, which are usually denoted as 'a' and 'c'. The d-spacing in the tetragonal crystal is shown in equation (10),

$$\frac{1}{d^2} = \frac{h^2+k^2+l^2}{a^2} + \frac{l^2}{c^2}$$  \hspace{1cm} (10)

with $h$, $k$ and $l$ are plane’s dimensions on $x$, $y$ and $z$ axis, respectively [16]. Equation (10) is then compared with equation (2), so equation (11) is obtained.

$$\frac{h^2+k^2+l^2}{a^2} + \frac{l^2}{c^2} = \frac{4\sin^2 \theta}{\lambda^2}$$  \hspace{1cm} (11)

$$\sin^2 \theta - \frac{\lambda^2}{4a^2} \left( \frac{h^2+k^2+l^2}{a^2} + \frac{l^2}{c^2} \right) = 0$$  \hspace{1cm} (12)

By replacing zero in the equation above with error during measurement, according to what Cohen has derived, that is expressed as $D \sin^2 2\theta$ [15], equation (13) is obtained,

$$\sin^2 \theta - \frac{\lambda^2}{4a^2} \left( h^2+k^2 \right) - \frac{\lambda^2}{4c^2} \left( l^2 \right) = D \sin^2 2\theta$$  \hspace{1cm} (13)

$$\sin^2 \theta - \frac{\lambda^2}{4a^2} \left( h^2+k^2 \right) + \frac{\lambda^2}{4c^2} \left( l^2 \right) + D \sin^2 2\theta$$  \hspace{1cm} (14)

$$\sin^2 \theta = R \phi + S \chi + T \psi$$  \hspace{1cm} (15)
with \( R = \frac{\lambda^2}{4a^2}, S = \frac{\lambda^2}{4c^2}, T = \frac{D}{10}, \phi = h^2 + k^2, \chi = l^2 \) and \( \psi = 10\sin^2 2\theta \). Transform equation (15) into a linear matrix equation shown in equation (16).

\[
\begin{pmatrix}
\Sigma \phi \sin^2 \theta \\
\Sigma \chi \sin^2 \theta \\
\Sigma \psi \sin^2 \theta 
\end{pmatrix} =
\begin{pmatrix}
\Sigma \phi^2 & \Sigma \phi \chi & \Sigma \phi \psi \\
\Sigma \phi \chi & \Sigma \chi^2 & \Sigma \chi \psi \\
\Sigma \phi \psi & \Sigma \chi \psi & \Sigma \psi^2
\end{pmatrix}
\begin{pmatrix}
R \\
S \\
T
\end{pmatrix}
\]  

(16)

Solution of the equation above can be found using the Cramer method. This is Cramer-Cohen method for tetragonal crystal structure.

2.2. Algorithm of the program

The algorithm used in this program is the Cramer-Cohen method. When the program runs, the program will ask the user to type in the code of crystal structure (1 for cubic and 2 for tetragonal). After that, user to type in the number of rows of the x-ray diffraction data. Then, the diffraction angles and miller indices have to be input by the user one by one. The program will process the inputs with Cramer-Cohen method according to the structure. As the output, the program will display the result of the lattice parameter calculation also its crystal structure’s characteristics.
3. Result and Discussions

The final output of this research is the code-based program. Using Python as the programming language and Cramer-Cohen method as the algorithm, the program runs accurately to analysing lattice parameter of XRD data.

3.1. User interface of the program

This program is created through Google Collaboratory service, a cloud service based on Jupyter Notebook provided by Google. This service can be used for programming in various languages, including Python. Therefore, the program that has been created can be accessed on a PC or smartphone as long as the program files are accessible and the internet network is available. Usage of different version of browsers does not affect the calculation results obtained, but may provide a different user experience and affect the length of time it takes to run the program. User interface in Microsoft Edge 91.0.864.48 version is shown in Figure 2.
The user has to be careful while inputting $hkl$ and diffraction angle value from the XRD data. Data should be inputted according to the format shown in the initial program instruction. If any inputted data is wrong or not as same as the format, the program will stop at the time and the user should reinput the data from the beginning. It is well-tolerated if this program compared to Microsoft Excel, because this program does not need multiple file according to the structure. It only needs a file and the code structure, then the program will analyse the XRD data smoothly.

3.2. Evaluation test for the program’s performance

The program is tested for analysing the diffraction angle and the miller index to determine the lattice parameter of the sample. The literature data of lattice parameter of these samples were taken from the International Centre for Diffraction Data (ICDD) [17].
Table 1. Results of lattice parameter measured by the program.

| Crystal Structure | Sample | Lattice Parameter (Å) | a | c |
|-------------------|--------|-----------------------|---|---|
| Cubic (a = b = c) | Cesium Chloride (CsCl) | Lit<sup>a</sup> | 4.123 | 4.123 |
|                   | Barium Strontium Titanate Oxide (Ba<sub>0.5</sub>Sr<sub>0.5</sub>TiO<sub>3</sub>) | Lit<sup>a</sup> | 3.947 | 3.947 |
|                   | Cadmium Telluride (CdTe) | Lit<sup>a</sup> | 6.481 | 6.482 |
|                   | Nickel (Ni) | Mea<sup>b</sup> | 3.524 | 3.524 |
|                   | NiO (Nickel Oxide) | Mea<sup>b</sup> | 4.194 | 4.194 |
|                   | CaO (Calcium Oxide) | Mea<sup>b</sup> | 4.810 | 4.811 |
|                   | CdS (Cadmium Sulfide) | Mea<sup>b</sup> | 5.818 | 5.818 |
| Tetragonal (a = b ≠ c) | Zirconium Oxide (ZrO<sub>2</sub>) | Lit<sup>a</sup> | 3.598 | 3.599 |
|                   | Copper Selenium Telluride (Cu<sub>2</sub>TeSe<sub>4</sub>) | Lit<sup>a</sup> | 5.449 | 5.459 |
|                   | Silver Indium (AgIn<sub>2</sub>) | Lit<sup>a</sup> | 6.869 | 6.870 |
|                   | Lithium Iron Oxide (Li<sub>2</sub>Fe<sub>2</sub>O<sub>4</sub>) | Lit<sup>a</sup> | 4.049 | 4.049 |
|                   | Chromium Tungsten Oxide (Cr<sub>2</sub>W<sub>2</sub>O<sub>8</sub>) | Lit<sup>a</sup> | 4.580 | 4.580 |

<sup>a</sup> Literature data from ICDD [17].

<sup>b</sup> Result provided by the program.

As seen from the results above, the percentage of error of the calculation result that program provide is extremely low. The percentage of error is less than 0.2 percent. It means that this program is very accurate for analysing lattice parameter of XRD data and also can be an alternative tool that is easier to use compared to the existing tools, such as Microsoft Excel.

4. Conclusion
A python-based program for calculating lattice parameter of cubic and tetragonal crystal structures has been successfully created using the Cramer-Cohen method as the algorithm. This program is created using the Google Collaboratory service, so it can be accessed through a PC or smartphone as long as the program’s file is accessible and the internet access is available. This program is very accurate and can be an efficient tool for analysing lattice parameter.

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