INDEXING THE X-RAY DIFFRACTION PATTERNS OF CUBIC AND HEXAGONAL STRUCTURES USING SPREADSHEETS

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ABSTRACT

X-Ray diffractometry is one of the most useful nondestructive techniques used to characterize crystalline substances. One can gain knowledge of structures and structural parameters, phases and texture, average grain size, crystalline strain, and defects, from an XRD pattern. In this study, we develop a macro-enabled Microsoft excel spreadsheet to study x-ray diffraction patterns. Through this spreadsheet x-ray diffraction patterns of materials can be analyzed to find the Miller indices and the lattice parameters. One must provide only the 2θ values for all the peaks, and then a single click on the calculate button gives the *'hkl'* values for all the peaks. This spreadsheet can be used to index *XRD* patterns of cubical and hexagonal structures.

Keywords: crystal structure, Miller indices, lattice planes, spreadsheets.

INTRODUCTION

Several researchers have explored the use of spreadsheets as educational tools across various fields. For instance, Smith et al. [1] demonstrated the effectiveness of integrating spreadsheets into mathematics education, highlighting their versatility in visualizing mathematical concepts, and fostering active learning. In the context of science education, Jones et al. [2] investigated the use of spreadsheets in chemistry classrooms, emphasizing their role in data analysis, modeling, and simulation exercises. Similarly, Brown and Miller [3] explored the integration of spreadsheets in physics education, highlighting their utility in conducting virtual experiments, analyzing experimental data, and reinforcing theoretical concepts. These studies collectively underscore the potential of spreadsheets as versatile and accessible educational tools that facilitate hands-on learning, data visualization, and problem-solving skills development across various disciplines.

Researchers have employed various methods for analyzing X-ray diffraction (XRD) patterns beyond the utilization of spreadsheets. One prominent approach involves the use of specialized software packages tailored for XRD data analysis, such as FullProf [4] and MAUD [5], which offer advanced functionalities for phase identification, peak fitting, and structural refinement. Additionally, advancements in machine learning techniques have enabled the development of algorithms for automated phase identification and quantitative analysis of XRD patterns [6]. Furthermore, studies have explored novel methodologies, including synchrotron X-ray diffraction and neutron diffraction, to elucidate complex material structures and phase transitions with high precision and accuracy [7,8]. These diverse approaches underscore the multifaceted nature of XRD analysis and highlight the importance of leveraging advanced techniques to unravel the structural properties of materials for various scientific and technological applications.

1 MATHEMATICAL BACKGROUND

The internal arrangement of atoms in a crystal structure determines the qualitative analysis and distinctive characteristics of a substance. A crystalline substance's crystal structure, which is a particular configuration of atoms or molecules, is crucial in determining physical properties including band structure and optical clarity. X-ray crystallography is thought to be the best method for precisely determining molecule structure at atomic precision. The detailed structural information provided by the crystallographic analysis paved the door for quick development in geology, minerals, seismology, nanotechnology, medicine, and other areas.

Atomic structure and X-ray diffraction pattern are closely related. Spectral lines from both atoms and ions make up this pattern. Thus, a sample's components can be determined using x-ray diffraction. The likelihood of the atomic or molecular transition decides the strength of the spectral line in the x-ray diffraction pattern. The sample's crystal structure can be determined using the x-ray diffraction pattern. While the intensity of a diffraction peak defines the atomic position within the cell and atomic number, its position determines the size and shape of the unit cell. A wide range of substances, including metals, liquids, polymers, minerals, plastics, catalysts, medicines, semiconductors, solar cells, ceramics, thin-film coatings, are analyzed using XRD patterns.

In this study, we have developed an *MS Excel VBA* program to analyze the x-ray diffraction patterns. With the help of this program, x-ray diffraction patterns can be examined to find the type of crystal structure and to find the lattice parameters. Spreadsheets give pupils the opportunity to practice dealing with actual data. Spreadsheets enable hypothetical analysis and give real-world examples to make theoretical or sophisticated theories understandable. One efficient technique to improve teaching effectiveness is for instructors to use Excel to turn any spreadsheet into a web page and share it with students. [9]

METHODS OF ANALYZING THE XRD PATTERNS

There are four methods, two for each (i.e., for cubic and hexagonal) structure, to find the Miller indices, and the lattice parameters. We will discuss all these one by one.

1.1 CUBIC STRUCTURES

1.1.1 Ratios' Method for Cubical Structures

To figure out the crystal structure of an unknown sample, we must find the Miller indices and the lattice parameters. The inter-planar spacing *d,* the distance between adjacent planes in the set *'hkl'* of a material with a cubic structure, and lattice parameter *a* can be obtained from the equation,

$$\frac{1}{d^2} = \frac{(h^2+k^2+l^2)}{a^2} \quad (1)$$

Using Bragg's law, the above equation becomes,

$$\sin^2\theta = \left(\frac{\lambda^2}{4a^2}\right)(h^2 + k^2 + l^2) \quad (2)$$

Solving equation (2) for a^2 gives,

$$a^2 = \left(\frac{\lambda^2}{4\sin^2\theta}\right)(h^2 + k^2 + l^2) \quad (3)$$

Thus, $\lambda^2/4a^2$ is different for different patterns, it can be seen that $\sin^2\theta$ is proportional to $h^2 + k^2 + l^2$ i.e., for increasing θ, planes with a higher *hkl* will diffract.

Writing equation (2) for two different sets of *hkl*, and dividing we get,

$$\boldsymbol{\sin^2\theta_1/\sin^2\theta_2 = \left(h_1^2 + k_1^2 + l_1^2\right)/\left(h_2^2 + k_2^2 + l_2^2\right)} \quad (4)$$

In a cubic system, the first reflections occur due to diffraction from the planes with the Miller indices *100* for primitive cubic, *110* for bcc, and *111* for fcc lattices, so $h^2 + k^2 + l^2 = 1, 2, \text{or } 3,$ respectively. Since, the ratio of $\sin^2\theta$ values for different planes, scales with the ratio of $h^2 + k^2 + l^2$ values, according to equation (4), and since, *h, k, & l* are always integers, the values of $h^2 + k^2 + l^2$ can always be found by dividing the $\sin^2\theta$ by the smallest (i.e., $\sin^2\theta_{\min}$ for *100*), and multiplying those ratios thus by a suitable integer to find values close to integers. Therefore, the values of $\sin^2\theta$ computed for all the XRD peaks are divided by the smallest one (first reflection). These ratios, if are not already, yield integers when multiplied by 2 or 3, etc. Those resulting numbers represent the values of $h^2 + k^2 + l^2$; hence, the *hkl* can easily be identified from the quadratic forms of Table-2. Alternatively, one may also index the XRD pattern using the ratio of $1/d^2$ values. Because θ is a directly measurable quantity, we have chosen to use the $\sin^2\theta$ values instead of $1/d^2$.

The lattice parameter a can be calculated from equation (3) as:

$$\boldsymbol{a = \frac{\lambda}{2\sin^2\theta}\sqrt{h^2 + k^2 + l^2}} \quad (5)$$

Using equation (5) we can completely index the diffraction pattern and find out the Bravais lattice and lattice parameters of any cubic crystal structure.

Identification of the Bravais Lattice

The identification of the Bravais lattice can be done by observing the systematic occurrence (or lack) of reflections in a diffraction pattern. The selection rules for cubic lattices are summarized in Table-1. The values of $h^2 + k^2 + l^2$ for the different cubic lattices follow specific sequences as shown below. [10]

Primitive cubic lattice: 1, 2, 3, 4, 5, 6, 8, 9, 10, 11, 12, 13, 14, 16, ...

Body-centered cubic lattice: 2, 4, 6, 8, 10, 12, 14, 16, ...

Face-centered cubic lattice: 3, 4, 8, 11, 12, 16, 19, 20, 24, 27, 32, ...

Table-1: *Selection Rules for the Presence or Absence of Reflections*

Bravais Lattice	Reflections Present for	Reflections Absent for
Primitive	All	None
Body-centered	even *h+k+l*	odd *h+k+l*
Face-centered	unmixed *h, k,* and *l* (all even, or all odd)	mixed *h, k,* and *l*

Table-2: *Quadratic Forms of Miller Indices for the Cubic System*

$h^2+k^2+l^2$	h	k	l	$h^2+k^2+l^2$	h	k	l	$h^2+k^2+l^2$	h	k	l	$h^2+k^2+l^2$	h	k	l
1	*1*	*0*	*0*	*29*	*4*	*3*	*2*	*51*	*5*	*5*	*1*	*75*	*5*	*5*	*5*
2	*1*	*1*	*0*	*29*	*5*	*2*	*0*	*51*	*7*	*1*	*1*	*75*	*7*	*5*	*1*
3	*1*	*1*	*1*	*30*	*5*	*2*	*1*	*52*	*6*	*4*	*0*	*76*	*6*	*6*	*2*
4	*2*	*0*	*0*	*32*	*4*	*4*	*0*	*53*	*6*	*4*	*1*	*77*	*6*	*5*	*4*
5	*2*	*1*	*0*	*33*	*4*	*4*	*1*	*53*	*7*	*2*	*0*	*78*	*7*	*5*	*2*
6	*2*	*1*	*1*	*33*	*5*	*2*	*2*	*54*	*5*	*5*	*2*	*81*	*6*	*6*	*3*
8	*2*	*2*	*0*	*34*	*4*	*3*	*3*	*54*	*6*	*3*	*3*	*81*	*7*	*4*	*4*
9	*2*	*2*	*1*	*34*	*5*	*3*	*0*	*54*	*7*	*2*	*1*	*83*	*7*	*5*	*3*
9	*3*	*0*	*0*	*35*	*5*	*3*	*1*	*56*	*6*	*4*	*2*	*85*	*7*	*6*	*0*
10	*3*	*1*	*0*	*36*	*4*	*4*	*2*	*57*	*5*	*4*	*4*	*86*	*6*	*5*	*5*
11	*3*	*1*	*1*	*36*	*6*	*0*	*0*	*57*	*7*	*2*	*2*	*86*	*7*	*6*	*1*
12	*2*	*2*	*2*	*37*	*6*	*1*	*0*	*58*	*7*	*3*	*0*	*88*	*6*	*6*	*4*
13	*3*	*2*	*0*	*38*	*5*	*3*	*2*	*59*	*5*	*5*	*3*	*89*	*7*	*6*	*2*
14	*3*	*2*	*1*	*38*	*6*	*1*	*1*	*59*	*7*	*3*	*1*	*90*	*7*	*5*	*4*
16	*4*	*0*	*0*	*40*	*6*	*2*	*0*	*61*	*6*	*4*	*3*	*94*	*7*	*6*	*3*
17	*3*	*2*	*2*	*41*	*4*	*4*	*3*	*61*	*6*	*5*	*0*	*97*	*6*	*6*	*5*
17	*4*	*1*	*0*	*41*	*5*	*4*	*0*	*62*	*6*	*5*	*1*	*98*	*7*	*7*	*0*
18	*3*	*3*	*0*	*41*	*6*	*2*	*1*	*62*	*7*	*3*	*2*	*99*	*7*	*5*	*5*
18	*4*	*1*	*1*	*42*	*5*	*4*	*1*	*65*	*6*	*5*	*2*	*99*	*7*	*7*	*1*
19	*3*	*3*	*1*	*43*	*5*	*3*	*3*	*65*	*7*	*4*	*0*	*101*	*7*	*6*	*4*
20	*4*	*2*	*0*	*44*	*6*	*2*	*2*	*66*	*5*	*5*	*4*	*102*	*7*	*7*	*2*
21	*4*	*2*	*1*	*45*	*5*	*4*	*2*	*66*	*7*	*4*	*1*	*107*	*7*	*7*	*3*
22	*3*	*3*	*2*	*45*	*6*	*3*	*0*	*67*	*7*	*3*	*3*	*108*	*6*	*6*	*6*
24	*4*	*2*	*2*	*46*	*6*	*3*	*1*	*68*	*6*	*4*	*4*	*110*	*7*	*6*	*5*
25	*4*	*3*	*0*	*48*	*4*	*4*	*4*	*69*	*7*	*4*	*2*	*114*	*7*	*7*	*4*
25	*5*	*0*	*0*	*49*	*6*	*3*	*2*	*70*	*6*	*5*	*3*	*121*	*7*	*6*	*6*
26	*4*	*3*	*1*	*49*	*7*	*0*	*0*	*72*	*6*	*6*	*0*	*123*	*7*	*7*	*5*
26	*5*	*1*	*0*	*50*	*5*	*4*	*3*	*73*	*6*	*6*	*1*	*134*	*7*	*7*	*6*
27	*3*	*3*	*3*	*50*	*5*	*5*	*0*	*74*	*7*	*4*	*3*	*147*	*7*	*7*	*7*
27	*5*	*1*	*1*	*50*	*7*	*1*	*0*	*74*	*7*	*5*	*0*				

To check if the spreadsheet works properly, we used the XRD pattern of aluminum, taken from page no. *102* of [10]. We plugged in the 2θ values only, and by single click on the calculate button, the whole table has been generated which is shown in the figure-1 below. The resulting table gives the lattice planes (*hkl)* and the lattice parameter (*a*) for cubical structures.

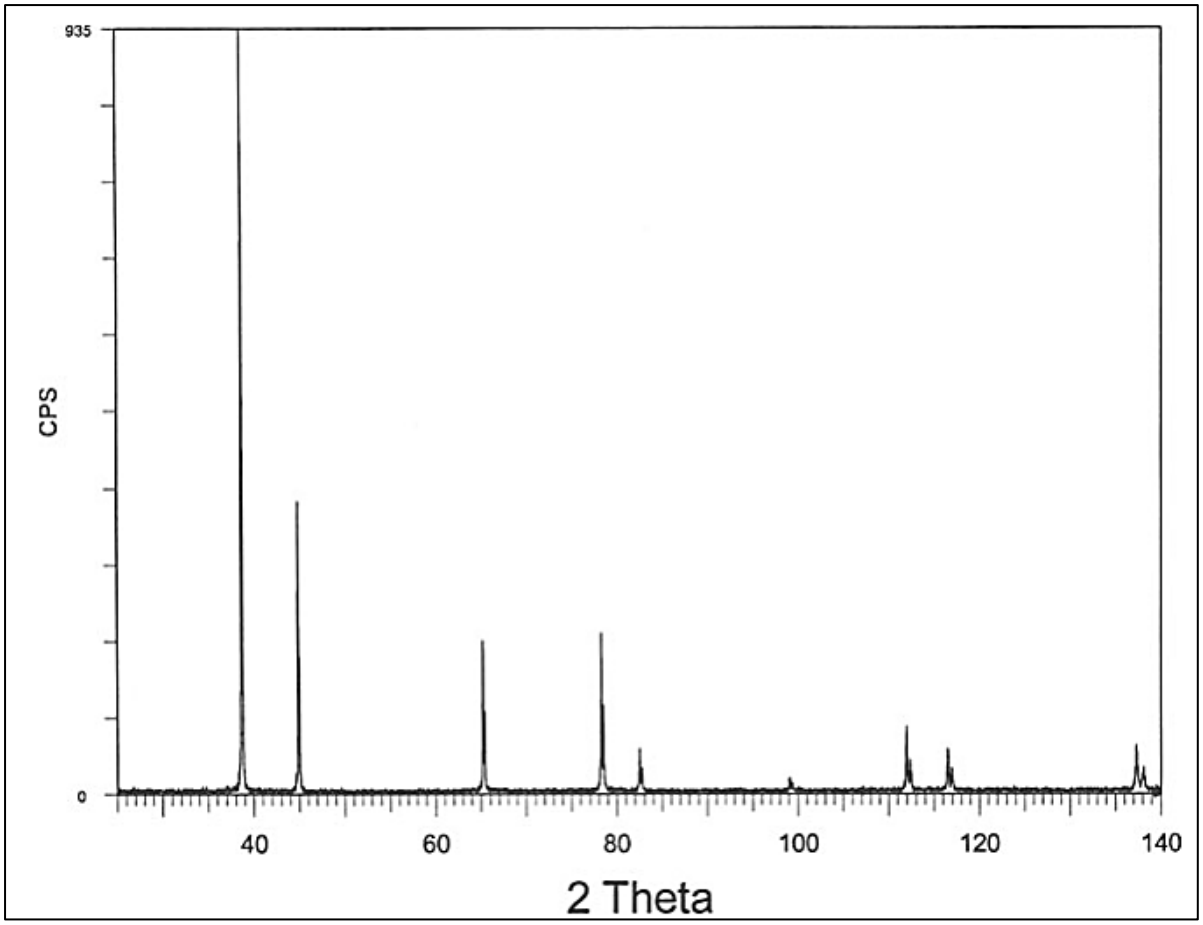


Figure-1 X-ray diffraction pattern of aluminum, taken from *page number 81* of [10].

	A	B	C	D	E	F	G	H	I	J	K	L	M
1	*Peak No.*	*2 θ*	*θ*	*Sin θ*	*Sin² θ*	*(Sin² θ)/(Sin² θ min)*	*3x(Sin² θ)/(Sin² θ min)*	*h²+k²+l²*	*h,k,l*	*a (nm)*	*Structure*		
2	1	38.52	19.260	0.3299	0.1088	1.000	3.000	3	*1,1,1*	0.40447	face-centred cubic		Calculate
3	2	44.76	22.380	0.3807	0.1450	1.332	3.997	4	*2,0,0*	0.40461			
4	3	65.14	32.570	0.5383	0.2898	2.663	7.990	8	*2,2,0*	0.40471			
5	4	78.26	39.130	0.6311	0.3983	3.660	10.981	11	*3,1,1*	0.40482			
6	5	82.47	41.235	0.6591	0.4345	3.993	11.980	12	*2,2,2*	0.40481			
7	6	99.11	49.555	0.7610	0.5792	5.323	15.969	16	*4,0,0*	0.40486			
8	7	112.03	56.015	0.8292	0.6875	6.319	18.957	19	*3,3,1*	0.40492			
9	8	116.60	58.300	0.8508	0.7239	6.653	19.959	20	*4,2,0*	0.40488			
10	9	137.47	68.735	0.9319	0.8685	7.982	23.946	24	*4,2,2*	0.40493			
11													
12										0.40478			

Figure-2 Screenshot of the spreadsheet based on the ratios method to find Miller indices of cubic crystals.

1.1.2 Analytical Method for Cubical Structures

An analytical method is also used to index the diffraction patterns in the same way. Starting from the first step, which is the same, we have already calculated the $\sin^2\theta$ values for all the major diffracted lines. In this method again, we will use the same equation as we have used above considering:

$$\sin^2\theta = \left(\frac{\lambda^2}{4a^2}\right)(h^2 + k^2 + l^2) \qquad (6)$$

We observe that $\sin^2\theta$ is proportional to $(h^2 + k^2 + l^2)$ after realizing that $\lambda^2/4a^2$ is a constant for any pattern, which we here refer to as A.

$$\boldsymbol{A = \left(\frac{\lambda^2}{4a^2}\right)} \tag{7}$$

The equation (6) will become,

$$\boldsymbol{\sin^2\theta = A(h^2 + k^2 + l^2)} \tag{8}$$

The possible values for $(h^2 + k^2 + l^2)$ in a simple cubic system are (*1,2,3,4,5,6,7,8,…*). To determine the required value of A, the observed values for each peak in the diffraction pattern are divided by (*2,3,4,5,6,…*) to obtain the common quotient. Dividing the $\sin^2\theta$ by the value of A, we can determine the '*hkl*'. Additionally, by simply rearranging the equation (7), one can find the lattice parameter as,

$$\boldsymbol{a = \frac{\lambda}{2\sqrt{A}}} \tag{9}$$

An analytical method can be used to index the diffraction pattern of any cubic crystal structure; the results are identical to those from the prior method. We can fully index the diffraction pattern of an unknown crystal structure using these two techniques, identify the Bravais lattices, and find the lattice parameters. Also, the nature of cubic crystal structure (whether *fcc* or *bcc)* can be identified.

The '*hkl*' values for the cubicle system are checked first; if they do not satisfy, we evaluate the values for the hexagonal system. The screenshot of the spreadsheet which uses the analytical method to find Miller indices of cubic crystals is shown in figure-2 below. We plugged in the values of 2θ only and the whole table-is generated by clicking one time on the calculate button. Here, we used XRD pattern of aluminum taken from page no. *102* of reference [10].

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	*Peak No.*	*2 θ*	*θ*	*Sin θ*	*Sin² θ*	*(Sin² θ)/2*	*(Sin² θ)/3*	*(Sin² θ)/4*	*(Sin² θ)/5*	*(Sin² θ)/6*	*(Sin² θ)/7*	*(Sin² θ)/8*	*(Sin² θ)/A*	*h²+k²+l²*	*h,k,l*	*Structure*
2	1	38.52	19.260	0.3299	0.1088	0.0544	0.0363	0.0272	0.0218	0.0181	0.0155	0.0136	3.0223	3	*1,1,1*	*face-centred cubic*
3	2	44.76	22.380	0.3807	0.1450	0.0725	0.0483	0.0362	0.0290	0.0242	0.0207	0.0181	4.0269	4	*2,0,0*	
4	3	65.14	32.570	0.5383	0.2898	0.1449	0.0966	0.0724	0.0580	0.0483	0.0414	0.0362	8.0500	8	*2,2,0*	
5	4	78.26	39.130	0.6311	0.3983	0.1991	0.1328	0.0996	0.0797	0.0664	0.0569	0.0498	11.0629	11	*3,1,1*	Calculate
6	5	82.47	41.235	0.6591	0.4345	0.2172	0.1448	0.1086	0.0869	0.0724	0.0621	0.0543	12.0688	12	*2,2,2*	
7	6	99.11	49.555	0.7610	0.5792	0.2896	0.1931	0.1448	0.1158	0.0965	0.0827	0.0724	16.0879	16	*4,0,0*	
8	7	112.03	56.015	0.8292	0.6875	0.3438	0.2292	0.1719	0.1375	0.1146	0.0982	0.0859	19.0985	19	*3,3,1*	
9	8	116.60	58.300	0.8508	0.7239	0.3619	0.2413	0.1810	0.1448	0.1206	0.1034	0.0905	20.1078	20	*4,2,0*	
10	9	137.47	68.7350	0.9319	0.868	0.434	0.289	0.2171	0.1737	0.1447	0.1241	0.1086	24.1239	24	*4,2,2*	
11																
12																

Figure-3 Screenshot of the spreadsheet using the analytical method to find Miller indices of cubic crystals.

1.2 Hexagonal Structures

1.2.1 Direct Method for Hexagonal Structures

Many common materials, which include semiconductor crystalline polymers, and several metals, have a hexagonal crystal structure. Suppose the diffraction pattern is expected to be the

hexagonal crystal system. In that case, the axial ratio c/a is given, and again the first step is to calculate the $\sin^2\theta$ values for all the major diffracted lines. To find the Miller indices and lattice parameters, the plane spacing equation for the hexagonal structure is.

$$\frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2+hk+k^2}{a^2}\right) + \frac{l^2}{c^2} \tag{10}$$

From Bragg's law ($\lambda = 2d\sin\theta$) we have,

$$\frac{1}{d^2} = \frac{4\sin^2\theta}{\lambda^2} \tag{11}$$

Comparing the above two equations we have,

$$\frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2+hk+k^2}{a^2}\right) + \frac{l^2}{c^2} = \frac{4\sin^2\theta}{\lambda^2} \tag{12}$$

Rearranging the above equation gives,

$$\sin^2\theta = \frac{\lambda^2}{4}\left[\frac{4}{3}\left(\frac{h^2+hk+k^2}{a^2}\right) + \frac{l^2}{c^2}\right] \tag{13}$$

As the axial ratio (c/a) for the hexagonal structures is usually given, the above equation after modification can be expressed as,

$$\sin^2\theta = \frac{\lambda^2}{4a^2}\left[\frac{4}{3}(h^2 + hk + k^2) + \frac{l^2}{(c/a)^2}\right] \tag{14}$$

From equation (14), the $\sin^2\theta$ has two components; the first of which includes the '*h*' and '*k*' values and the second of which includes the '*l*' values. The value of the two components $\left(\frac{4}{3}\right)(h^2 + hk + k^2)$ and $l^2/(c/a)^2$ for different sets of '*h*', '*k*' and '*l*' are given in the Table-3 and Table-4 respectively, taken from pages *126-127* of [10].

Table-3: values of $(4/3)(h^2 + hk + k^2)$

h	*k*	*0*	*1*	*2*	*3*
0		0.0000	1.3333	5.3333	12.0000
1		1.3333	4.0000	9.3333	17.3333
2		5.3333	9.3333	16.0000	25.3333
3		12.0000	17.3333	25.3333	36.0000

Table-4: values of $l^2/(c/a)^2$ for zinc $(c/a = 1.8563)$

l	0	1	2	3	4	5	6
l^2	0	2	4	9	16	25	36
$l^2/(c/a)^2$	0.0000	0.2902	1.1608	2.6118	4.6432	7.2550	10.4472

Now, we can add both the components from Table-3 and table-4 and arrange them in the possible combinations for different *'hkl'* values in increasing order for all the values. The

structure factor of hexagonal structures suggests that reflections are absent when the following two conditions are satisfied. [10]

1. When $h+2k = 3N$ (where N is an integer).
2. When l is odd.

All the remaining reflections will be present. The values of 'a' and 'c' in hexagonal structures have different values, the indices 'h' and 'k' can be swapped, but the index 'l' cannot. In this manner, the Miller indices for different values of 'hkl' can be found. The lattice parameters 'a' and 'c' can be calculated using equation (14).

The value of 'a' can be found using '$hk0$' reflections. For this, substituting $l = 0$ in equation (14) we get,

$$\boldsymbol{\sin^2\theta = \frac{\lambda^2}{4a^2}\left[\frac{4}{3}(h^2 + hk + k^2)\right]} \tag{15}$$

Rearranging equation (15) for 'a' gives,

$$\boldsymbol{a^2 = \frac{\lambda^2}{3\sin^2\theta}(h^2 + hk + k^2)} \tag{16}$$

Taking square root on both sides to get 'a'

$$\boldsymbol{a = \frac{\lambda}{\sqrt{3}\sin^2\theta}\sqrt{(h^2 + hk + k^2)}} \tag{17}$$

To calculate the value of 'c' we use the reflections of '$00l$' type. Using $h=k=0$ in the equation (14) we have,

$$\boldsymbol{\sin^2\theta = \frac{\lambda^2}{4a^2}\left(\frac{l^2}{(c/a)^2}\right)} \tag{18}$$

Rearranging equation (18) for 'c' gives,

$$\boldsymbol{c^2 = \frac{\lambda^2}{4\sin^2\theta}l^2} \tag{19}$$

Taking square root on both sides to get 'c'

$$\boldsymbol{c = \frac{\lambda}{4\sin\theta}l} \tag{20}$$

The values of 'a' and 'c' can be calculated in this way, and we can completely index the diffraction pattern of the hexagonal crystal and find the Bravais lattice.

To check if the spreadsheets work properly, we used the XRD pattern of zinc taken from *page number 130* of [10]. Once again, we plugged in the 2θ values for the XRD peaks of the zinc. After clicking on the calculate button we got the lattice planes (*hkl*), and the lattice parameters (*a* and *c*) as shown in the figure-3 below.

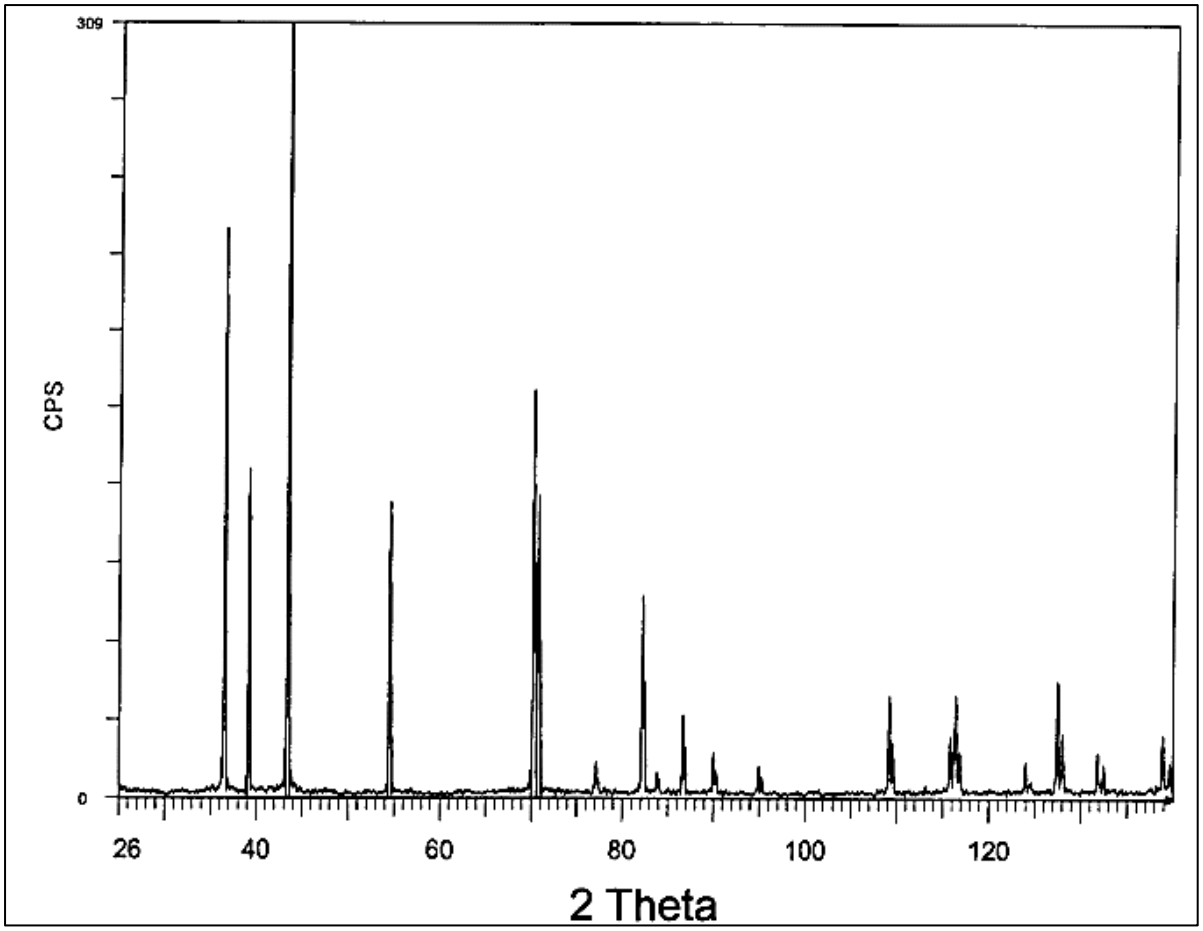


Figure-4 X-ray diffraction patter of zinc-taken from *page number 130* of [10]

	A	B	C	D	E	F	G	H	I	J	K	L
1	***Peak No.***	***2 θ***	***θ***	***Sin θ***	***Sin^2 θ***	***(4/3)[h^2+hk+k^2]+[l^2/(c/a)^2]***	***h,k,l***	$a = \frac{\lambda}{\sqrt{3}\sin\theta}\sqrt{h^2+hk+k^2}$ nm	$c = \frac{\lambda}{2\sin\theta}l$ nm		***c/a***	***1.8563***
2	1	36.31	18.16	0.3116	0.0971	1.1614	***0,0,2***		0.4944		***λ***	***1.54E-10***
3	2	38.98	19.49	0.3336	0.1113	1.3313	***1,0,0***	0.2666			***a***	***2.664E-10***
4	3	43.21	21.61	0.3682	0.1356	1.6219	***1,0,1***					
5	4	54.32	27.16	0.4565	0.2084	2.4927	***1,0,2***				Calculate	
6	5	70.08	35.04	0.5741	0.3296	3.9424	***1,0,3***					
7	6	70.64	35.32	0.5781	0.3342	3.9974	***1,1,0***	0.2665				
8	7	77.04	38.52	0.6228	0.3879	4.6397	***0,0,4***		0.4947			
9	8	82.09	41.05	0.6567	0.4313	5.1588	***1,1,2***					
10	9	83.72	41.86	0.6673	0.4453	5.3263	***2,0,0***	0.2666				
11	10	86.54	43.27	0.6854	0.4698	5.6193	***2,0,1***					
12	11	89.91	44.96	0.7066	0.4993	5.9722	***1,0,4***					
13	12	94.88	47.44	0.7366	0.5426	6.4901	***2,0,2***					
14	13	109.13	54.57	0.8148	0.6639	7.9410	***2,0,3***					
15	14	115.80	57.90	0.8471	0.7176	8.5833	***1,0,5***					
16	15	116.37	58.19	0.8498	0.7222	8.6383	***1,1,4***					
17	16	124.03	62.02	0.8831	0.7799	9.3285	***2,1,0***	0.2665				
18	17	127.47	63.74	0.8968	0.8043	9.6203	***2,1,1***					
19	18	131.86	65.93	0.9130	0.8336	9.9708	***2,0,4***					
20	19	138.56	69.28	0.9353	0.8748	10.4636	***0,0,6***		0.4941			
21	20	139.14	69.57	0.9371	0.8782	10.5042	***2,1,2***					
22												

Figure-5 Screenshot of the spreadsheet using the direct method to find Miller indices of hexagonal crystals.

1.2.2 Analytical Method for Hexagonal Structures

Another method is an analytical method used to find the crystal structure of the hexagonal close-packed structure. An analytical method is effective and holds less error, and less time-consuming than the earlier used method. The method we have used first can sometimes be tricky in finding *'hkl'* values to calculate $\sin^2\theta$ values. Sometimes, the diffracted lines peak is very weak, and it is impossible that you have missed a peak while seeing 2θ values. This will cause an error in all the *'hkl'* values and give you the wrong answer for the lattice parameter. Therefore, for this purpose, an alternate method which is an analytical method, is also used to index the pattern of hexagonal structure. Since we again use equation (14),

$$\boldsymbol{\sin^2\theta = \frac{\lambda^2}{4a^2}\left[\frac{4}{3}(h^2 + hk + k^2) + \frac{l^2}{(c/a)^2}\right]} \quad (21)$$

The above equation can be changed to,

$$\boldsymbol{\sin^2\theta = A(h^2 + hk + k^2) + Cl^2} \quad (22)$$

where, $A = \lambda^2/3a^2$, and $C = \lambda^2/4c^2$ (23)

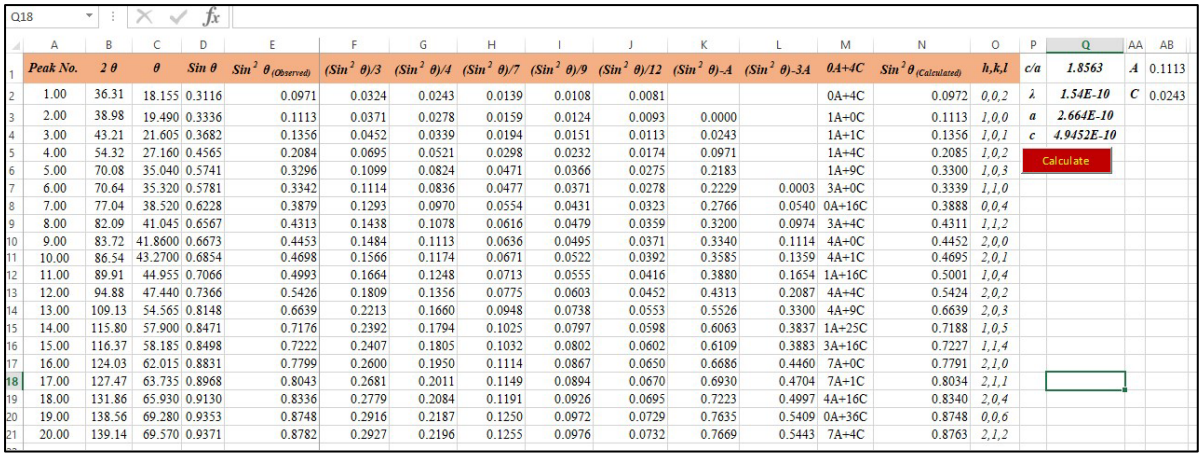
We use *hk0* (*l=0*) type reflections to find the value of *A*. Therefore, the permitted values of *h* and *k* for $(h^2 + hk + k^2)$ are *1, 3, 4, 7, 9, 12, ...* as shown in Table-3. In the first step we divide all the $\sin^2\theta$ values by *1, 3, 4, 7, 9, 12, ...* and find the common quotient. Hence, the least common recurring value will yield the value of *A*. Then, we use $A = \lambda^2/3a^2$ to find '*a*' for all the $\sin^2\theta$ values.

Then we use equation (22), after rearranging, to find the value of *C*,

$$\boldsymbol{Cl^2 = \sin^2\theta - A(h^2 + hk + k^2)} \quad (24)$$

For a hexagonal crystal, '*l*' can only have integer values 1,2,3,…, and for $l^2 = 1,4,9, \ldots$, we can find *C* with the help of *00l* type reflection as already mentioned in the earlier section. To get the value of *C*, we subtract (*A,3A,4A,7A,...*) from each $\sin^2\theta$ to get the remainder of the order (*1,4,9,...*) which will be the *00l* type reflections. Again, the common repeated value gives the value of *C*, and the lattice parameters *c* can be found using the relation $C = \lambda^2/4c^2$. Using the proper combination of *A* and *C*, by choosing the *'hkl'* values allowed by structure factor, we indexed the entire pattern and used the equation (23) to find the value of *a* and *c*.

Again, to check if the spreadsheet works properly, we used the XRD pattern of zinc taken from *page number 130* of [10]. Plugging in the 2θ values for the XRD peaks of the zinc, clicking on the calculate button, we got the lattice planes (*hkl*), and the values of *A* and *C* as shown in the figure-3 below.



Peak No.	2θ	θ	Sin θ	$Sin^2\theta_{(Observed)}$	$(Sin^2\theta)/3$	$(Sin^2\theta)/4$	$(Sin^2\theta)/7$	$(Sin^2\theta)/9$	$(Sin^2\theta)/12$	$(Sin^2\theta)$-A	$(Sin^2\theta)$-3A	0A+4C	$Sin^2\theta_{(Calculated)}$	h,k,l
1.00	36.31	18.155	0.3116	0.0971	0.0324	0.0243	0.0139	0.0108	0.0081			0A+4C	0.0972	0,0,2
2.00	38.98	19.490	0.3336	0.1113	0.0371	0.0278	0.0159	0.0124	0.0093	0.0000		1A+0C	0.1113	1,0,0
3.00	43.21	21.605	0.3682	0.1356	0.0452	0.0339	0.0194	0.0151	0.0113	0.0243		1A+1C	0.1356	1,0,1
4.00	54.32	27.160	0.4565	0.2084	0.0695	0.0521	0.0298	0.0232	0.0174	0.0971		1A+4C	0.2085	1,0,2
5.00	70.08	35.040	0.5741	0.3296	0.1099	0.0824	0.0471	0.0366	0.0275	0.2183		1A+9C	0.3300	1,0,3
6.00	70.64	35.320	0.5781	0.3342	0.1114	0.0836	0.0477	0.0371	0.0278	0.2229	0.0003	3A+0C	0.3339	1,1,0
7.00	77.04	38.520	0.6228	0.3879	0.1293	0.0970	0.0554	0.0431	0.0323	0.2766	0.0540	0A+16C	0.3888	0,0,4
8.00	82.09	41.045	0.6567	0.4313	0.1438	0.1078	0.0616	0.0479	0.0359	0.3200	0.0974	3A+4C	0.4311	1,1,2
9.00	83.72	41.8600	0.6673	0.4453	0.1484	0.1113	0.0636	0.0495	0.0371	0.3340	0.1114	4A+0C	0.4452	2,0,0
10.00	86.54	43.2700	0.6854	0.4698	0.1566	0.1174	0.0671	0.0522	0.0392	0.3585	0.1359	4A+1C	0.4695	2,0,1
11.00	89.91	44.955	0.7066	0.4993	0.1664	0.1248	0.0713	0.0555	0.0416	0.3880	0.1654	1A+16C	0.5001	1,0,4
12.00	94.88	47.440	0.7366	0.5426	0.1809	0.1356	0.0775	0.0603	0.0452	0.4313	0.2087	4A+4C	0.5424	2,0,2
13.00	109.13	54.565	0.8148	0.6639	0.2213	0.1660	0.0948	0.0738	0.0553	0.5526	0.3300	4A+9C	0.6639	2,0,3
14.00	115.80	57.900	0.8471	0.7176	0.2392	0.1794	0.1025	0.0797	0.0598	0.6063	0.3837	1A+25C	0.7188	1,0,5
15.00	116.37	58.185	0.8498	0.7222	0.2407	0.1805	0.1032	0.0802	0.0602	0.6109	0.3883	3A+16C	0.7227	1,1,4
16.00	124.03	62.015	0.8831	0.7799	0.2600	0.1950	0.1114	0.0867	0.0650	0.6686	0.4460	7A+0C	0.7791	2,1,0
17.00	127.47	63.735	0.8968	0.8043	0.2681	0.2011	0.1149	0.0894	0.0670	0.6930	0.4704	7A+1C	0.8034	2,1,1
18.00	131.86	65.930	0.9130	0.8336	0.2779	0.2084	0.1191	0.0926	0.0695	0.7223	0.4997	4A+16C	0.8340	2,0,4
19.00	138.56	69.280	0.9353	0.8748	0.2916	0.2187	0.1250	0.0972	0.0729	0.7635	0.5409	0A+36C	0.8748	0,0,6
20.00	139.14	69.570	0.9371	0.8782	0.2927	0.2196	0.1255	0.0976	0.0732	0.7669	0.5443	7A+4C	0.8763	2,1,2

c/a	1.8563	A	0.1113
λ	1.54E-10	C	0.0243
a	2.664E-10		
c	4.9452E-10		

Calculate

Figure-6 Screenshot of the spreadsheet designed for the analytical method to find Miller indices of hexagonal crystals.

2 RESULTS AND DISCUSSIONS

2.1 Cubic structures

Figure-2 and Figure-3 show the screenshots of the spreadsheets developed for the identification of the cubic crystals using the ratios method and the analytical method, respectively. Our spreadsheet also identifies the Bravais lattice, and gives the value of the lattice constant, as in the case of aluminum, it is face-centered cubic having the lattice constant value equal to 0.40478 nm, which can be seen in the screenshots of Figure 2 and Figure 3. The values of *hkl* found by both methods for the XRD pattern of aluminum are shown in Table-1 below.

Table 1: Miller indices for pure aluminum found by both the ratios method and the analytical method.

Peak No.	*2θ*	*$h^2+k^2+l^2$*	*h,k,l*	*a (nm)*
1	38.52	3	*1,1,1*	0.40447
2	44.76	4	*2,0,0*	0.40461
3	65.14	8	*2,2,0*	0.40471
4	78.26	11	*3,1,1*	0.40482
5	82.47	12	*2,2,2*	0.40481
6	99.11	16	*4,0,0*	0.40486
7	112.03	19	*3,3,1*	0.40492
8	116.60	20	*4,2,0*	0.40488
9	137.47	24	*4,2,2*	0.40493

2.2 Hexagonal structures

Figure-5 and Figure-6 show the screenshots of the spreadsheets developed for the identification of the hexagonal crystals using the direct method and the analytical method, respectively. In

the direct method (Figure-5) you only need to provide the values of *c/a*, and λ, and the spreadsheet will do the rest of the calculations and will give the values of *a*, *c*, and the Miller indices. In the analytical method (Figure-6) you need to provide the values of *c/a*, either *c* or *a*, and λ, and the spreadsheet will give the value of the other i.e., *a* or *c*, and the Miller indices. The values of *a* and *c* for zinc are found to be 2.664 Å and 4.945 Å, respectively.

The values of *hkl* found by both methods for the XRD pattern of zinc are shown in Table-2 below.

Table 1: Miller indices for pure zinc found by both the methods.

Peak No.	***2θ***	***h,k,l***
1	36.31	*0,0,2*
2	38.98	*1,0,0*
3	43.21	*1,0,1*
4	54.32	*1,0,2*
5	70.08	*1,0,3*
6	70.64	*1,1,0*
7	77.04	*0,0,4*
8	82.09	*1,1,2*
9	83.72	*2,0,0*
10	86.54	*2,0,1*
11	89.91	*1,0,4*
12	94.88	*2,0,2*
13	109.13	*2,0,3*
14	115.80	*1,0,5*
15	116.37	*1,1,4*
16	124.03	*2,1,0*
17	127.47	*2,1,1*
18	131.86	*2,0,4*
19	138.56	*0,0,6*
20	139.14	*2,1,2*

3 CONCLUSION

In this study, we have developed a user-friendly macro-enabled Microsoft Excel spreadsheet for the analysis of XRD patterns. The spreadsheet allows for the determination of Miller indices and lattice parameters of cubic and hexagonal crystal structures. The accuracy of the spreadsheet was demonstrated by comparing the calculated values with literature values for various samples. The spreadsheet provides a simple and efficient tool for researchers and students to analyze XRD patterns and gain insights into the crystal structure of materials.

3.1 Future work

There are some other modules given in [10] which can also be programmed in the same way as we did for the identification of the cubic and hexagonal structures in the current work. In

future work, the spreadsheet can be further improved by incorporating additional functionalities such as peak fitting, background subtraction, and phase identification. Additionally, the spreadsheet can be extended to analyze XRD patterns of other crystal systems such as tetragonal, orthorhombic, and monoclinic structures.

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