DETERMINATION OF LATTICE PARAMETERS OF MgB2 SUPERCONDUCTOR WITH HEXOGONAL CRYSTAL STRUCTURE

PROJECT REPORT

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DEPARTMENT OF PHYSICS

CERTIFICATE

Certificate that the document titled "DETERMINATIONOF LATTICE PARAMETERS OFMGB2SUPERCONDUCTOR WITH HEXAGONAL CRYSTAL STRUCTURE" is a bona-fide of the project report presented by AKHIL V (university reg.no:200021036514) of sixth semester BSc Physics, model I submitted In partial fulfillment of the requirements for the award of the degree of Bachelor Of Science In physics (Model - I) of the Mahatma Gandhi university, Kottayam during the academic year 2020-2023.

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INTRODUCTION

Certain materials show certain unique properties like complete banishment of natural electrical resistance and the magnetic flux is pushed out of the material. All the materials showing these properties are considered as superconductors. In an ordinary metallic conductor when resistance decreases slowly as the temperature gets lowered but a superconductor has a characteristic critical temperature below which the resistance drops abruptly to zero. Electric current through a superconducting loop wire can keep on moving for an unspecified without any power source.

The superconductivity phenomenon was discovered in 1911 by Heike Kamerlingh Onnes. Just like ferromagnetism and atomic spectral lines, superconductivity can only be explained using quantum mechanics. Materials to materials all the physical properties of the superconductors changes, i.e. the value of the superconducting gap, the critical temperature, magnetic field and the current density at which the property known as superconductivity is destroyed. Superconductors are the best electromagnets. They are used in MRI machines, mass spectrometers etc. The most sensitive magnetometers Josephson junctions which are the building blocks of SQUIDs (superconducting quantum interference devices) are build using superconductors.

In Superconductors MgB2 (Magnesium Diboride) is an inorganic compound. It is a dark gray, water-insoluble solid. The compound has attracted attention because it becomes superconductor at 39 K (−234 °C). In terms of its composition, MgB2 differs from most of the low-temperature superconductors, which feature mainly transition metals. Its superconducting mechanism is primarily described by BCS theory. Its superconducting properties was found in 2001. Its critical temperature (T_c) of 39 K (−234 °C; −389 °F) is the highest amongst conventional superconductors. Its electronic structure is such that there exist

two types of electrons at the Fermi level with widely differing behaviors, one of them (sigma-bonding) being much more strongly superconducting than the other (pi-bonding).

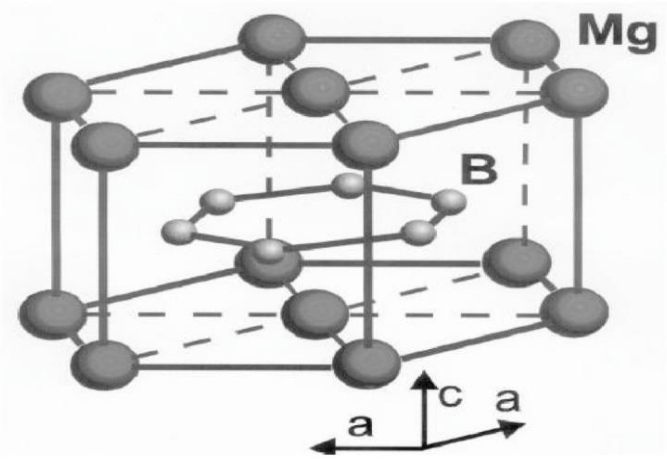
The simplest synthesis involves high temperature reaction between boron and magnesium powders. Formation begins at 650 °C; however, since magnesium metal melts at 652 °C, the reaction may involve diffusion of magnesium vapor across boron grain boundaries. To minimize these, we synthesis it in a both end sealed stainless-steel tube preventing the formation of MgO_2. Properties depends on the composition and manufacturing processes of MgB2. Many properties are anisotropic due to the layered structure.MgB2 is a multi-band superconductor, that is each Fermi surface has different superconducting energy gap. For MgB2 s-wave superconducting gap is large due because the sigma bond of boron is strong and the pi bond is weak and produces small s-wave gap. MgB2 is a brittle material.

Simple chemical reactions between B and Mg can produce MgB2, usually at temperatures over Mg's melting point of 650 °C. Using the Powder in Sealed Tube (PIST) method of in situ solid state synthesis, bulk MgB2 samples were created bar after heating

In order to remove the formed MgB2 core, the samples' edges were ground for structural and Characterizations of superconductivity. The standard sample containers were then filled with the powder samples, and ambient conditions were used to record the XRD data. After that, phase identification and lattice parameter calculations were performed on the acquired XRD data. In this project's the provided X-Ray diffraction pattern, lattice properties of MgB2 were calculated using the standard relation for the p6/mmmm space group hexagonal crystal structure.

THEORY

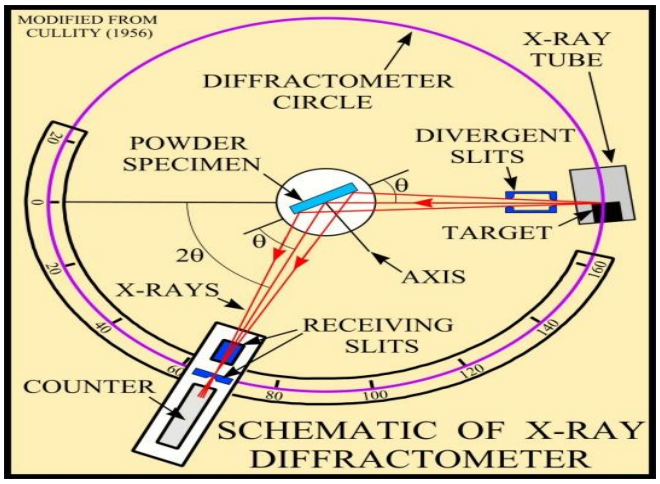
A Hexagonal ALB2 type crystal structure with a P6/mmm space group. The boron atoms are located like a honeycomb structure. The mg atoms are located with a closed packed layer. MgB2 shows a complex bonding structure they consist of ionic inter layer bonding and covalent bonding the unit cell of MgB2 consists of four magnesium and eight boron atoms are located in it. Mg is completely ionized in MgB2.The valence electron of the mg atoms donates to the boron planes forming a ionic bond using the boron atoms. The boron and magnesium are stabilized in their structure and ionic charge transfer MgB2 in boron is exhibits a graphene like layer of hexagon while bulk boron is stable in a rhombohedral phase also the distance between the MgB2 layer of mg-mg atoms is considerably smaller than that of bulk mg. Magnesium transfer the valence electron to boron layers. Filling of boron in 2pz orbitals by reducing the mg-mg bonding distance due to the outer most shell is empty. Polycrystalline MgB2 has a grain size of 10 nm – 10 μm.



X-rays are electromagnetic radiation with a wavelength significantly shorter than that of light. They are an x-ray tube schematic cross section. formed when sufficiently energetic electrically charged particles are slowed down. The high voltage that is maintained across the electrodes

in an X-ray tube attracts electrons to a metal target (the anode). At the site of impact, X-rays are generated and radiate in all directions. For geological purposes, copper-targeted tubes are frequently utilised because they emit their highest characteristic radiation (K1) at a wavelength of roughly 1.5 angstroms.

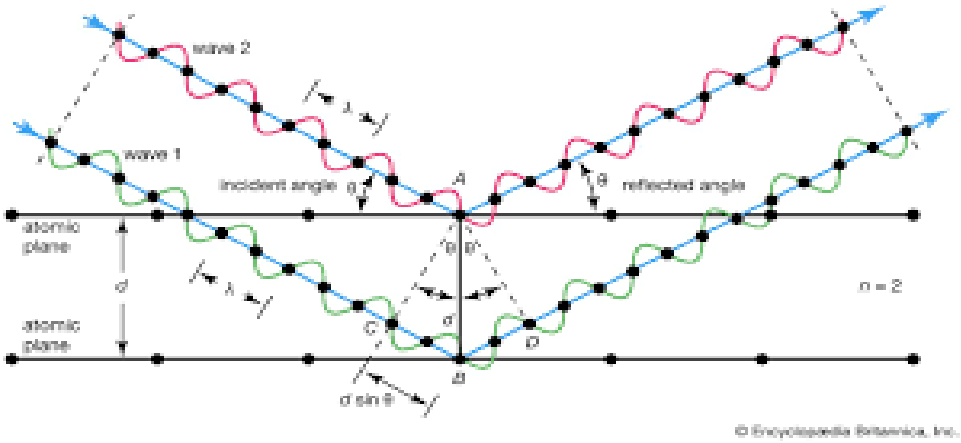
A source of monochromatic radiation and an X-ray detector placed on the edge of a graded circle centred on the powder specimen make up the fundamental geometry of an X-ray diffractometer. Divergent slits reduce background noise, collimate the radiation, and restrict scattered (non-diffracted) radiation when they are placed between the X-ray source and the specimen and between the specimen and the detector. A goniometer is mechanically connected to the detector and specimen holder so that a fixed 2:1 ratio of the detector and specimen rotation through 2x degrees and x degrees occurs.



The X-ray powder diffraction technique is the most convenient and easy method for the phase identification of crystalline materials. This technique has been widely employed to examine the phase formation, lattice parameters, strain and grain size. XRD data can also be used for a semi- quantitative phase analysis. In the current work, the materials' powder XRD patterns were collected using a Philips X'pert Pro (PW 3040/60) X-ray diffractometer with CuK (= 1.540566) radiation and a custom detector called the X-ray diffraction detector. On the side of the diffracted beam, an X'Celerator and a monochromator. The device has fully automated operation and data using Bragg-Brentano geometry acquisition. The X-ray beam was constrained to the target area via programmable slits designated sampling region. The majority

of the scans were done through a tube voltage of 40kV and 30mA, respectively. Samples used were a scan of 20° to 80° (2θvalues) with a 0.02° step size.It takes roughly 20 minutes to scan. The samples were either bulk or wire core samples fully powdered into a fine powder. The standard sample containers were then filled with the powder samples, and ambient conditions were used to record the XRD data. Considering that there is less powder (particularly from thinner wires). A typical zero backdrop holder was utilised (diameter).After that, phase identification and lattice parameter calculations were performed on the acquired XRD data. The lattice parameter estimates for MgB2 were done using the d values of a few chosen peaks. As the sample and detector rotate through their respective angles, the amount of diffracted X-rays is continually measured. When the mineral has lattice planes with the proper d-spacing to diffract X-rays at that value of, the intensity peaks. At low values of 2, the peak positions overlap even though each peak is made up of two distinct reflections (K1 and K2), with K2 appearing as a hump on the side of K1. Higher values of result in more separation. Usually, these merged peaks are regarded as a single peak. The centre of the peak at 80% peak height is commonly used to determine the 2 position of the diffraction peak.Results are often displayed as X-ray counts (intensity) and peak positions at 2 in the form of a table or an x-y plot. The intensity (I) is either expressed as the intensity at the peak above the background or as the integrated intensity in the region beneath the peak. The ratio of the peak intensity to the intensity of the peak with the highest peak is used to calculate the relative intensity (relative intensity = I/I1 x 100).

Reflection phenomenon take place when monochromatic X-rays fall on a crystal. When The angle of incidence has certain values which depends on the lattice parameters of the crystal only then this reflection takes place as shown in the figure given below.



Sir W. H. Bragg and his son Sir W. L. Bragg developed a relation between the angle of incidence and the wavelength using the equation, **nλ = 2d sinθ** to explain why the crystal faces reflect the X-ray beams at certain angles of incidence Θ. The distance between atomic layers in a crystal is denoted as d and the variable lambda λ gives the wavelength of the incident X-ray beam and n is the order of reflection which is an integer. The reflection corresponding to n=1,2,3,4,5, etc. are referred to as first order, second order, third order, fourth order, fifth order etc. As the order of reflection increases the intensity decreases.

From the X-ray diffraction pattern certain peaks of MgB2 are used to determine the d values from which the lattice parameters are determined. Lattice parameters were calculated for the hexagonal crystal structure of space group p6/mmm, using the relation:

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

where a and c are the lattice parameters that we need to find out, d values and miller indices values (hkl) are given in X-ray diffraction pattern.

An XRD peak's full width at half maximum (FWHM) is influenced by a variety of variables, including crystal size, lattice strain, instrument parameters, and others. For qualitatively

evaluating MgB2 peaks, the FWHM of selected peaks was employed. the grain size and lattice strain. Williamson-Hall plot analysis. The lattice strain and crystallite size was calculated using (FWHM x cosθ versus sinθ) from the slope and the y-intercept, respectively.

EXPERIMENTAL SETUP AND PROCEDURE

The powder in sealed tube method, also known as in situ solid state synthesis, is used to create MgB2 polycrystalline samples.For this mixing, stainless steel tubes that can withstand temperatures as high as 900 degrees Celsius are required. Using a hydraulic press, the tube's one end is compressed entirely, leaving no room for air to enter. Using an electronic balance, the stochiometric masses of boron and magnesium powder were measured. Using a mortar made of agate and a pestle, the powders are combined and ground. The open end of the stainless steel tube with the previously pressed end is entirely filled with this powder mixture. The open end is likewise sealed after filling. To prevent magnesium vapours from escaping during heating, the end sealing is always completed by welding. These powdered combinations are heated in the air directly for a predetermined period of time at a rate of 5 degrees Celsius per minute, between 600 and 900 degrees Celsius, with time allotted for furnace cooling. The bar-shaped MgB2 core is removed from samples by grinding the edges, and the stainless steel sheath was mechanically peeled off for structural characterizations.

The most popular and straightforward approach for identifying the phase of crystalline formations was X-ray powder diffraction. It is frequently used to look at the grain size, strain, and lattice characteristics. The samples' XRD patterns utilising a CuKa (1.540566) x-ray defractometer and a monochromater on the deffracted beam side. Programable slits were employed to confine the X-ray beam to specified locations, and the procedure was carried out at a voltage and current of 40 kV and 30 mA. The temperature range for the samples was 20 to 80 degrees. A scan lasts for roughly 20 minutes. Samples are collected in sample holders, and XRD data are collected. Lattice parameter calculations were then performed using these XRD data.

In our project, the XRD graphed in a graph and the d values of particular peaks of MgB2 are used to calculate the lattice parameters.

Lattice parameters were calculated using these equation

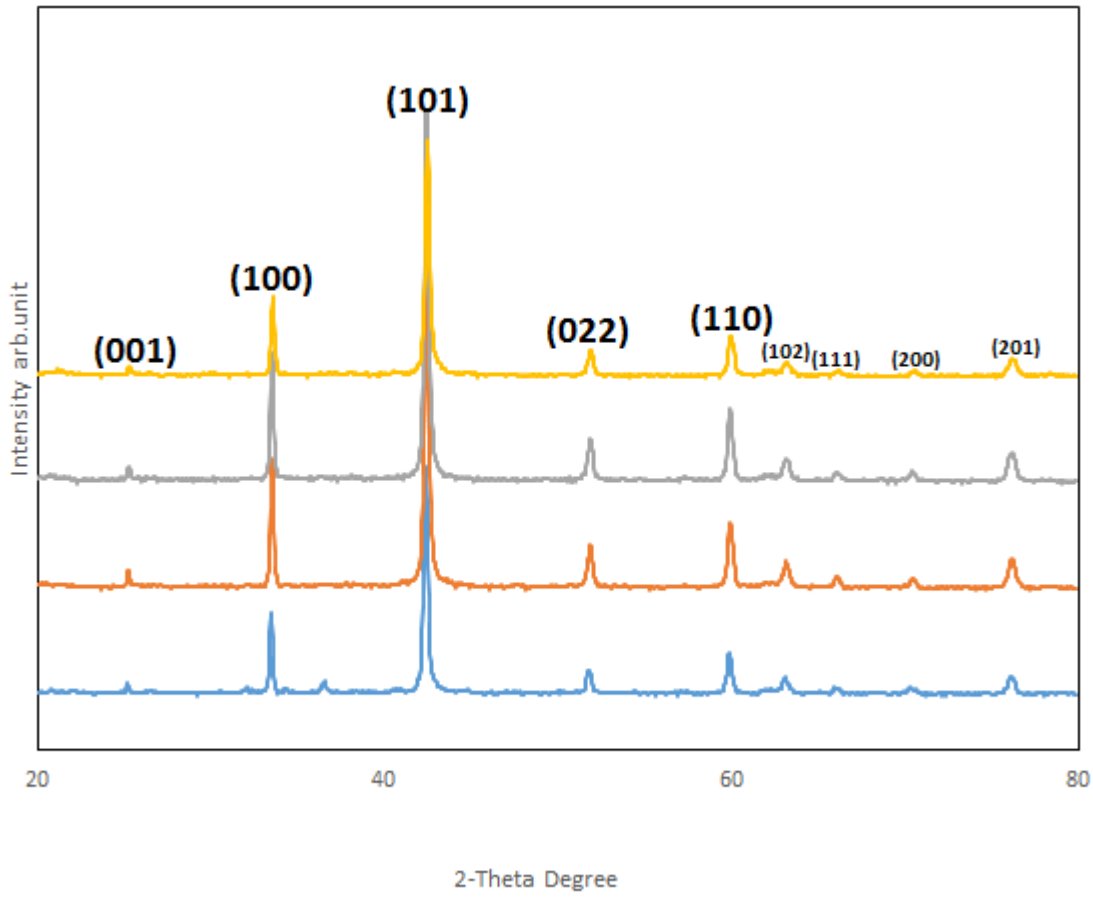
$$\frac{1}{d^2} = \frac{4(h^2+hk+k^2)}{3a^2} + \frac{l^2}{c^2}$$

where h, k and l are miller indices values, d is inter planar spacing and a and c are the lattice parameters whose value to be found out.

The values of the miller indices and the d values are substituted into this equation, which is implemented in the C++ computer language, and the output is the lattice parameters a and c. We acquire several a and c values, whose mean value is determined, for each miller index and d value.

OBSERVATIONS

From the X-ray powder diffraction method, we plot a graph as follows:



From X-ray, the wavelength of Cu Kα is given by;

λ=1.541 Å Using

Braggs law,

$d=(n\lambda)/(2\sin\theta)$

n=1 (First order)

From the graphical data,

λ (Å)	**(hkl)**	**2θ (º)**	**Θ (º)**	**d=(nλ)/2sinθ (Å)**
1.541	(001)	25.22927	12.614635	d1 = 3.5280
	(100)	33.45122	16.72561	d2 =2.677
	(101)	42.37503	21.187515	d3 = 2.131
	(022)	51.86703	25.9335	d4 = 1.761
	(110)	59.88844	29.9442	d5 = 1.543
	(102)	63.16835	31.5841	d6 = 1.471
	(111)	66.17188	33.08594	d7 = 1.411
	(200)	70.41654	35.20827	d8 = 1.336
	(201)	76.19864	38.09932	d9 =1.248

Table 1.1

λ (Å)	**(hkl)**	**2θ (º)**	**Θ (º)**	**d=(nλ)/2sinθ (Å)**
1.541	(001)	25.3294	12.6647	d1 = 3.514
	(100)	33.5148	16.7574	d2 =2.672
	(101)	42.4418	21.2209	d3 = 2.091
	(022)	51.83361	25.9168	d4 = 1.732
	(110)	59.95529	29.9776	d5 = 1.542
	(102)	63.19727	31.5986	d6 = 1.470
	(111)	66.27215	33.1360	d7 = 1.409
	(200)	70.68392	35.3434	d8 = 1.331
	(201)	76.29891	38.1494	d9 = 1.247

Table 1.2

λ (Å)	**(hkl)**	**2θ (º)**	**Θ (º)**	**d=(nλ)/2sinθ (Å)**
1.541	(001)	25.39638	12.6981	d1 = 3.505
	(100)	33.51806	16.7590	d2 =2.672
	(101)	42.40846	21.2042	d3 = 2.130
	(022)	51.9338	25.9669	d4 = 1.759
	(110)	59.95529	29.9776	d5 = 1.542
	(102)	63.33096	31.66548	d6 = 1.467
	(111)	66.37472	33.18736	d7 = 1.407
	(200)	70.68392	35.3419	d8 = 1.331
	(201)	76.29891	38.1494	d9 = 1.247

Table 1.3

λ (Å)	**(hkl)**	**2θ (º)**	**Θ (º)**	**d=(nλ)/2sinθ (Å)**
11.54	(001)	25.59692	12.79846	d1 = 3.478
	(100)	33.61833	16.809165	d2 =2.664
	(101)	42.4753	21.23765	d3 = 2.127
	(022)	52.00072	26.00036	d4 = 1.757
	(110)	60.02213	30.0110	d5 = 1.540
	(102)	63.5315	31.5315	d6 = 1.473
	(111)	66.37242	33.18621	d7 = 1.407
	(200)	70.9513	35.47565	d8 = 1.327
	(201)	76.46002	38.23001	d9 = 1.245

Table 1.4

By using the equation $\frac{1}{d^2} = \frac{4(h^2+hk+k^2)}{3a^2} + \frac{l^2}{c^2}$ placed in the program we can calculate lattice parameter a and c.

PROGRAM

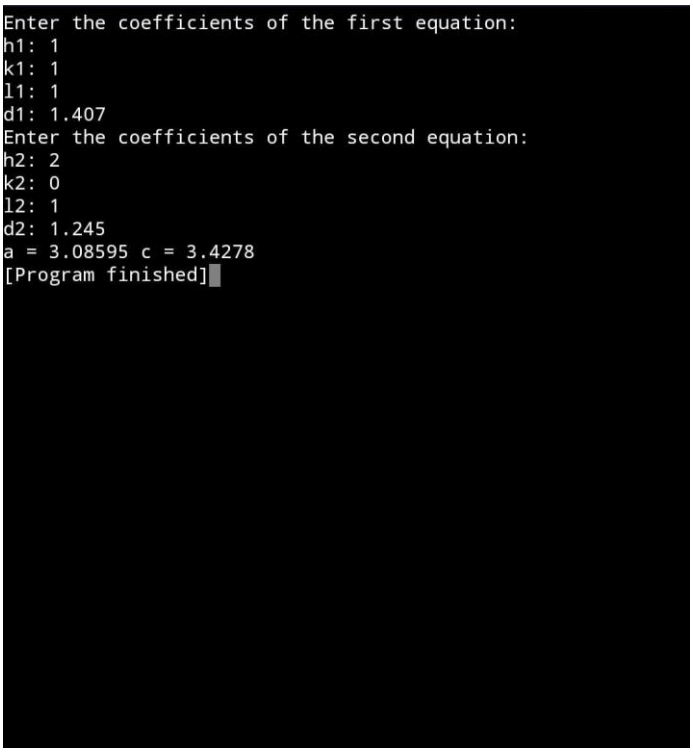
A tool for tackling mathematical problems, the programme described is written in the C++ programming language. It can offer a final solution to the issue based on user input and is made to solve difficult equations involving numerous variables.

The user provides the programme with input variables like h1, k1, l1, d1, h2, k2, l2, and d2. The equation that needs to be solved is represented by these values as various variables.

After receiving these inputs, the

programme performs a series of calculations to determine other variables' values, including c1, a1, , c2, a2, and The values of c1, a1 are determined in the first stage by using the input values as a guide. Based on particular equations that are connected to the input values, these computations are performed.

On the basis of the provided values for h2, k2, l2, and d2, the programme also determines c2, a2.



Source code:

```
#include <iostream>
#include <math.h>
using namespace std;
int main()
 {
double h1, k1, l1, d1, h2, k2, l2, d2,d_1,n,m,d_2 ;
double a1, b1, c1, a2, b2, c2, x, y;
cout << "Enter the coefficients of the first equation: " << endl;
cout << "h1: ";
cin >> h1;
cout << "k1: ";
cin >> k1;
cout << "l1: ";
cin >> l1;
cout << "d1: ";
cin >> d1;
cout << "Enter the coefficients of the second equation: " << endl;
cout << "h2: ";
cin >> h2;
cout << "k2: ";
cin >> k2;
cout << "l2: ";
cin >> l2;
cout << "d2: ";
cin >> d2;
c1 = 1/(d1*d1);
a1 = 4*((h1*h1) + (h1*k1) + (k1*k1))/3;
b1 = (l1*l1);
c2 = 1/(d2*d2);
a2 = 4*((h2*h2) + (h2*k2) + (k2*k2))/3;
b2 = (l2*l2);
x = (c2*b1-b2*c1)/(a2*b1-b2*a1);
y = (c1-a1*x)/b1;
long double a,c ;
a=1/(sqrt(x));
c=1/(sqrt(y));
cout << "a = " << a << " c = " << c ;
return 0
 }
```

LATTICE PARAMETERS OBTAINED FROM THE PROGRAM:

Intensity1:

(hkl)	d (Å)	$\frac{1}{d^2} = \frac{4(h^2+hk+k^2)}{3a^2} + \frac{l^2}{c^2}$	a (Å)	c (Å)
(001)	d1 = 3.5280	$1/d1^2 = 1/c^2$	-	3.528
(100)	d2 =2.677	$1/d2^2 = 4/3a^2$	3.09113	-
(101)	d3 = 2.131	$1/d3^2 = (4/3a^2) + (1/c^2)$	-	-
(002)	d4 = 1.761	$1/d4^2 = 4/c^2$	-	3.522
(110)	d5 = 1.543	$1/d5^2 = 4/a^2$	3.086	-
(102)	d6 = 1.471	$1/d6^2 = (4/3a^2) + (4/c^2)$	-	-
(111)	d7 = 1.411	$1/d7^2 = (4/a^2) + (1/c^2)$	-	-
(200)	d8 = 1.336	$1/d8^2 = 16/3a^2$	3.0853	
(201)	d9 =1.248	$1/d1^2 = 1/c^2$	-	-

(hkl)	d (Å)	$\frac{1}{d^2} = \frac{4(h^2+hk+k^2)}{3a^2} + \frac{l^2}{c^2}$	a (Å)	c (Å)
(101)	d3 = 2.131	$1/d3^2 = (4/3a^2) + (1/c^2)$	3.090	3.52138
(102)	d6 = 1.471	$1/d6^2 = (4/3a^2) + (4/c^2)$		
(101)	d3 = 2.131	$1/d3^2 = (4/3a^2) + (1/c^2)$	3.074	3.553
(111)	d7 = 1.411	$1/d7^2 = (4/a^2) + (1/c^2)$		
(101)	d3 = 2.131	$1/d3^2 = (4/3a^2) + (1/c^2)$	3.079	3.544
(201)	d9 =1.248	$1/d1^2 = 1/c^2$		
(102)	d6 = 1.471	$1/d6^2 = (4/3a^2) + (4/c^2)$	3.079	3.527
(111)	d7 = 1.411	$1/d7^2 = (4/a^2) + (1/c^2)$		
(102)	d6 = 1.471	$1/d6^2 = (4/3a^2) + (4/c^2)$	3.081	3.525
(201)	d9 =1.248	$1/d1^2 = 1/c^2$		
(111)	d7 = 1.411	$1/d7^2 = (4/a^2) + (1/c^2)$	3.088	3.47
(201)	d9 =1.248	$1/d1^2 = 1/c^2$		

Mean a= 3.083Å and Mean c= 3.523

Lattice Paramters:

a= 3.083Å

c= 3.523Å

Intensity 2:

(hkl)	d (Å)	$\frac{1}{d^2} = \frac{4(h^2+hk+k^2)}{3a^2} + \frac{l^2}{c^2}$	a (Å)	c (Å)
(001)	d1 = 3.514	$1/d1^2 = 1/c^2$	-	3.514
(100)	d2 =2.672	$1/d2^2 = 4/3a^2$	3.085	-
(101)	d3 = 2.091	$1/d3^2 = (4/3a^2) + (1/c^2)$	-	-
(002)	d4 = 1.732	$1/d4^2 = 4/c^2$	-	3.464
(110)	d5 = 1.542	$1/d5^2 = 4/a^2$	3.084	-
(102)	d6 = 1.470	$1/d6^2 = (4/3a^2) + (4/c^2)$	-	-
(111)	d7 = 1.409	$1/d7^2 = (4/a^2) + (1/c^2)$	-	-
(200)	d8 = 1.331	$1/d8^2 = 16/3a^2$	3.073	
(201)	d9 = 1.247	$1/d9^2 = (16/3a^2) + (1/c^2)$	-	-

(hkl)	d (Å)	$\frac{1}{d^2} = \frac{4(h^2+hk+k^2)}{3a^2} + \frac{l^2}{c^2}$	a (Å)	c (Å)
(101)	d3 = 2.091	$1/d3^2 = (4/3a^2) + (1/c^2)$	2.974	3.580
(102)	d6 = 1.470	$1/d6^2 = (4/3a^2) + (4/c^2)$		
(101)	d3 = 2.091	$1/d3^2 = (4/3a^2) + (1/c^2)$	3.114	3.331
(111)	d7 = 1.409	$1/d7^2 = (4/a^2) + (1/c^2)$		
(101)	d3 = 2.091	$1/d3^2 = (4/3a^2) + (1/c^2)$	3.106	3.332
(201)	d9 = 1.247	$1/d1^2 = 1/c^2$		
(102)	d6 = 1.470	$1/d6^2 = (4/3a^2) + (4/c^2)$	3.074	3.526
(111)	d7 = 1.409	$1/d7^2 = (4/a^2) + (1/c^2)$		
(102)	d6 = 1.470	$1/d6^2 = (4/3a^2) + (4/c^2)$	3.079	3.523
(201)	d9 = 1.247	$1/d1^2 = 1/c^2$		
(111)	d7 = 1.409	$1/d7^2 = (4/a^2) + (1/c^2)$	3.092	3.418
(201)	d9 = 1.247	$1/d1^2 = 1/c^2$		

Mean a=3.075Å and c=3.461Å

Lattice Paramters:

a= 3.075Å

c= 3.461Å

Intensity3:

(hkl)	d (Å)	$\frac{1}{d^2} = \frac{4(h^2+hk+k^2)}{3a^2} + \frac{l^2}{c^2}$	a (Å)	c (Å)
(001)	d1 = 3.505	$1/d1^2 = 1/c^2$	-	3.505
(100)	d2 =2.672	$1/d2^2 = 4/3a^2$	3.085	-
(101)	d3 = 2.130	$1/d3^2 = (4/3a^2) + (1/c^2)$	-	-
(002)	d4 = 1.759	$1/d4^2 = 4/c^2$	-	3.518
(110)	d5 = 1.542	$1/d5^2 = 4/a^2$	3.084	-
(102)	d6 = 1.467	$1/d6^2 = (4/3a^2) + (4/c^2)$	-	-
(111)	d7 = 1.407	$1/d7^2 = (4/a^2) + (1/c^2)$	-	-
(200)	d8 = 1.331	$1/d8^2 = 16/3a^2$	3.073	
(201)	d9 = 1.247	$1/d9^2 = (16/3a^2) + (1/c^2)$	-	-

(hkl)	d (Å)	$\frac{1}{d^2} = \frac{4(h^2+hk+k^2)}{3a^2} + \frac{l^2}{c^2}$	a (Å)	c (Å)
(101)	d3 = 2.130	$1/d3^2 = (4/3a^2) + (1/c^2)$	3.259	3.245
(102)	d6 = 1.467	$1/d6^2 = (4/3a^2) + (4/c^2)$		
(101)	d3 = 2.130	$1/d3^2 = (4/3a^2) + (1/c^2)$	3.060	3.579
(111)	d7 = 1.407	$1/d7^2 = (4/a^2) + (1/c^2)$		
(101)	d3 = 2.130	$1/d3^2 = (4/3a^2) + (1/c^2)$	3.076	3.546
(201)	d9 = 1.247	$1/d1^2 = 1/c^2$		
(102)	d6 = 1.467	$1/d6^2 = (4/3a^2) + (4/c^2)$	3.070	3.517
(111)	d7 = 1.407	$1/d7^2 = (4/a^2) + (1/c^2)$		
(102)	d6 = 1.467	$1/d6^2 = (4/3a^2) + (4/c^2)$	3.080	3.512
(201)	d9 = 1.247	$1/d1^2 = 1/c^2$		
(111)	d7 = 1.407	$1/d7^2 = (4/a^2) + (1/c^2)$	3.108	3.309
(201)	d9 = 1.247	$1/d1^2 = 1/c^2$		

Mean a=3.099Å and c=3.466Å

Lattice Paramters:

a= 3.099Å

c= 3.466Å

Intensity 4:

(hkl)	d (Å)	$\frac{1}{d^2} = \frac{4(h^2+hk+k^2)}{3a^2} + \frac{l^2}{c^2}$	a (Å)	c (Å)
(001)	d1 = 3.478	$1/d1^2 = 1/c^2$	-	3.478
(100)	d2 =2.664	$1/d2^2 = 4/3a^2$	3.076	-
(101)	d3 = 2.127	$1/d3^2 = (4/3a^2) + (1/c^2)$	-	-
(002)	d4 = 1.757	$1/d4^2 = 4/c^2$	-	3.514
(110)	d5 = 1.540	$1/d5^2 = 4/a^2$	3.08	-
(102)	d6 = 1.473	$1/d6^2 = (4/3a^2) + (4/c^2)$	-	-
(111)	d7 = 1.407	$1/d7^2 = (4/a^2) + (1/c^2)$	-	-
(200)	d8 = 1.327	$1/d8^2 = 16/3a^2$	3.064	
(201)	d9 = 1.245	$1/d9^2 = (16/3a^2) + (1/c^2)$	-	-

(hkl)	d (Å)	$\frac{1}{d^2} = \frac{4(h^2+hk+k^2)}{3a^2} + \frac{l^2}{c^2}$	a (Å)	c (Å)
(101)	d3 = 2.127	$1/d3^2 = (4/3a^2) + (1/c^2)$	3.074	3.536
(102)	d6 = 1.473	$1/d6^2 = (4/3a^2) + (4/c^2)$		
(101)	d3 = 2.127	$1/d3^2 = (4/3a^2) + (1/c^2)$	3.063	3.558
(111)	d7 = 1.407	$1/d7^2 = (4/a^2) + (1/c^2)$		
(101)	d3 = 2.127	$1/d3^2 = (4/3a^2) + (1/c^2)$	3.071	3.542
(201)	d9 = 1.245	$1/d1^2 = 1/c^2$		
(102)	d6 = 1.473	$1/d6^2 = (4/3a^2) + (4/c^2)$	3.066	3.540
(111)	d7 = 1.407	$1/d7^2 = (4/a^2) + (1/c^2)$		
(102)	d6 = 1.473	$1/d6^2 = (4/3a^2) + (4/c^2)$	3.071	3.537
(201)	d9 = 1.245	$1/d1^2 = 1/c^2$		
(111)	d7 = 1.407	$1/d7^2 = (4/a^2) + (1/c^2)$	3.085	3.427
(201)	d9 = 1.245	$1/d1^2 = 1/c^2$		

Mean a=3.072Å and c=3.516Å

Lattice Paramters:

a= 3.072 Å

c= 3.516 Å

RESULT

- Values of interplanar spacing (d) is listed below

Intensity1:

(hkl)	**d** (Å)
(001)	d1 = 3.5280
(100)	d2 =2.677
(101)	d3 = 2.131
(022)	d4 = 1.761
(110)	d5 = 1.543
(102)	d6 = 1.471
(111)	d7 = 1.411
(200)	d8 = 1.336
(201)	d9 =1.248

Intensity2:

(hkl)	**d** (Å)
(001)	d1 = 3.514
(100)	d2 =2.672
(101)	d3 = 2.091
(022)	d4 = 1.732
(110)	d5 = 1.542
(102)	d6 = 1.470
(111)	d7 = 1.409
(200)	d8 = 1.331
(201)	d9 = 1.247

Intensity3:

(hkl)	**d** (Å)
(001)	d1 = 3.505
(100)	d2 =2.672
(101)	d3 = 2.130
(022)	d4 = 1.759
(110)	d5 = 1.542
(102)	d6 = 1.467
(111)	d7 = 1.407
(200)	d8 = 1.331
(201)	d9 = 1.247

Intensity4:

(hkl)	**d** (Å)
(001)	d1 = 3.478
(100)	d2 =2.664
(101)	d3 = 2.127
(022)	d4 = 1.757
(110)	d5 = 1.540
(102)	d6 = 1.473
(111)	d7 = 1.407
(200)	d8 = 1.327
(201)	d9 = 1.245

- Lattice parameters obtained from different intensities:

Intensity1: a=3.083Å
c=3.523Å

Intensity2: a=3.075Å
c=3.461Å

Intensity3: a=3.099Å
c=3.466Å

Intensity4: a=3.072Å
c=3.512Å

CONCLUSION

The XRD-diffraction pattern data was utilised to get the d values, which were then used to determine the lattice parameters a and c using C++ programming.

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