ANALYSIS OF X-RAY DIFFRACTION PATTERN OF NANO CARON DOPED MgB_2 SUPERCONDUCTOR

PROJECT REPORT

submitted in partial fulfillment of the award of degree of

BACHELOR OF SCIENCE IN PHYSICS

(Model II – Computer Application)

OF

MAHATMA GANDHI UNIVERSITY, KOTTAYAM

BY

JOHN PAUL
CLASS NO: 20V1116
REGISTER N0: 200021039175

Under The Guidance Of

DEPARTMENT OF PHYSICS

BHARATA MATA COLLEGE, THRIKKAKARA, KOCHI-21

2020-23 BATCH

BHARATA MATA COLLEGE, THRIKKAKARA, KOCHI-21

DEPARTMENT OF PHYSICS

CERTIFICATE

*Certificate that this document titled "**ANALYSIS OF X-RAY DIFFRACTION PATTERN OF NANO CARON DOPED MgB_2 SUPERCONDUCTOR**" is a bona-fide of the project report presented by JOHN PAUL (university reg.no: 200021039175) of sixth semester BSc Physics, model II Computer application submitted In partial fulfillment of the requirements for the award of the degree of Bachelor Of Science In physics (Model - II Computer application) of the Mahatma Gandhi university, Kottayam during the academic year 2020-2023.*

Project Guide **Head of the department**

Dr. Neson Varghese

Internal Examiner **External Examiner**

CONTENT

INTRODUCTION

Superconductivity is a fascinating phenomenon that has captured the attention of scientists and engineers for decades. When a material is cooled below a certain temperature, it can lose all electrical resistance and exhibit perfect conductivity, leading to a range of potential technological applications.

In 1911, Heike Kamerlingh Onnes, a physicist from the Netherlands, made a groundbreaking discovery regarding superconductivity. He found that mercury, when cooled to extremely low temperatures near absolute zero (-273.15°C), displayed zero electrical resistance and conducted electricity without any energy loss. Superconductivity is characterized by the absence of resistance in materials, resulting in zero electrical resistance. The Meissner effect, which is the complete expulsion of magnetic fields from the material, is responsible for this phenomenon. This discovery revolutionized the field of physics and has since led to many important technological advancements.

When electrons move through a material in pairs, known as Cooper pairs, they can exhibit superconductivity, a phenomenon where electricity is conducted with zero resistance and no energy loss. Electrons are attracted to each other and form pairs due to an attractive force. However, at normal temperatures, this force is too weak to keep the electrons paired, causing them to move independently and collide with other particles. As a result, energy loss occurs due to these collisions. As the temperature of the material decreases, the thermal energy decreases as well, causing the formation of Cooper pairs and their movement without any resistance. This phenomenon is explained by the BCS theory, which was introduced by John Bardeen, Leon Cooper, and John Schrieffer in 1957. Superconductivity has many advantages, but its practical applications are currently restricted due to the fact that it only occurs at extremely low temperatures. For most superconductors, near absolute zero temperatures (-273.15°C) are required for them to function, making them costly to manufacture and challenging to work with. Despite these limitations, there are high-temperature superconductors that can operate at higher temperatures. These materials are not yet fully comprehended, but their discovery has

opened up new avenues for the practical utilization of superconductivity in the future.

In this context, we have selected MgB2 as the focus of our project. MgB2 is a superconductor that was discovered in 2001, and since then it has attracted a lot of attention due to its unique properties. One of the key advantages of MgB2 is its high transition temperature, which makes it easier to achieve superconductivity without having to cool the material to extremely low temperatures [MgB2 is a unique material that exhibits superconducting behavior at relatively high temperatures]. This has opened up new possibilities for practical applications of superconductivity, including energy-efficient power transmission, magnetic levitation, and high-speed computing. Another advantage of MgB2 is its relatively simple crystal structure, which makes it easier to study and manipulate than some other superconductors. This has allowed researchers to explore the fundamental mechanisms behind superconductivity in more detail, which may lead to new breakthroughs and innovations in the field.

Superconductivity is a unique phenomenon that occurs at very low temperatures, where some materials exhibit zero resistance to electrical current flow. This property has numerous practical applications, including the development of high-performance magnets, power transmission cables, and medical imaging devices. Magnesium diboride (MgB2) is a well-known superconducting material that has attracted significant attention due to its high critical temperature and simple crystal structure. In addition to its practical applications, MgB2 also has scientific significance as a research topic in its own right. The study of superconductivity is a highly active area of research, with many unanswered questions and challenges still to be overcome. By focusing on MgB2, we hope to contribute to this ongoing effort to understand and harness the unique properties of superconducting materials.

The process of synthesizing MgB2 involves reacting boron (B) powder with magnesium (Mg) at temperatures above 650°C, which is the melting point of Mg. This reaction leads to the formation of MgB2. One of the commonly used methods for synthesizing MgB2 is the solid-state reaction method called Powder in Sealed Tube (PIST).. This method involves the mixing of magnesium and boron powders in a stoichiometric ratio of 1:2, respectively. The mixture of B and Mg is sealed and then

placed in a tube with an inert gas, such as argon, and heated to a high temperature for a specified period. The reaction occurs within the sealed tube, and the resulting MgB2 is obtained in the form of bar-shaped core by grinding the edges of the sample.

During the solid-state reaction, the magnesium and boron powders react with each other to form magnesium boride (MgB4). This reaction is then followed by the formation of MgB2. The reaction takes place in stages and can take several hours to complete, depending on the reaction conditions. The reaction temperature and time must be optimized to ensure the formation of pure MgB2 without any undesired phases. The quality of the starting materials used is also essential to obtain high-quality MgB2 with minimal impurities. To obtain high-quality MgB2, the reaction should be carried out under an inert atmosphere such as argon or nitrogen. The use of an inert atmosphere helps to prevent the oxidation of the powders, which could lead to impurities in the final product. The graphite crucible used for the reaction should be clean and free from impurities that may affect the reaction. After the reaction is complete, the MgB2 powder is cooled to room temperature under an inert atmosphere before being removed from the furnace. The MgB2 powder obtained from the solid-state reaction method can be further processed using different techniques such as hot pressing or sintering. These techniques can help to improve the properties of the material, such as density, grain size, and homogeneity. MgB2 has potential applications in various fields such as energy storage, transportation, and medical imaging. The synthesis of high-quality MgB2 is crucial for the development of these applications.

To characterize the structure and superconducting properties of the MgB2 sample, X-ray diffraction (XRD) measurements were performed. The powder samples were filled in standard sample holders and the XRD data were recorded at ambient conditions. The XRD data were then analyzed to identify the phases present and to calculate the lattice parameters of MgB2. The hexagonal crystal structure of space group p6/mmm was assumed for this analysis. The lattice parameters of MgB2 were estimated using the standard relation for hexagonal crystal structures.

X-ray diffraction (XRD) is a powerful technique that is widely used to analyze the crystal structure and composition of materials. When X-rays are directed at a material, they interact with the atoms in the crystal lattice, leading to constructive interference and

the generation of a diffraction pattern. This diffraction pattern contains information about the spacing and orientation of the atoms within the crystal structure, which can be used to identify the crystal structure and the composition of the material. In the case of superconducting materials, the analysis of XRD patterns is particularly important because the structural properties of these materials are closely related to their superconducting behavior. Superconductors exhibit zero resistance to electrical current when they are cooled below a certain temperature, known as the critical temperature. This behavior is due to the unique arrangement of atoms in the crystal structure of the material, which allows for the unimpeded flow of electrons through the lattice. By analyzing the XRD patterns of superconducting materials, researchers can gain insights into the crystal structure and composition of these materials, which can help them to understand and optimize their superconducting properties.

In this project, we focus on the X-ray diffraction (XRD) analysis of pure MgB2 and its nano carbon-doped form, as XRD analysis is a powerful tool used to analyze the crystal structure and composition of materials, and is of particular interest when studying superconductors. The XRD analysis of these materials will provide insights into their structural properties, which are closely related to their superconducting behavior. The synthesis of pure MgB2 can be done simply by the reaction of B with Mg, while the doping of carbon in the material requires a more intricate process. The samples will then be analyzed using XRD, and the obtained data will be used to determine the phase identification and lattice parameter calculations of the materials. The results of this study will contribute to the understanding of the structural and superconducting properties of MgB2 and its carbon-doped form.

Carbon doping is a technique that is widely used in the field of materials science to modify the properties of various materials. The addition of carbon nanoparticles to a material can improve its mechanical, electrical, and thermal properties. This technique is also used to enhance the superconducting properties of certain materials, such as MgB2. This technique involves adding small amounts of carbon nanoparticles to the material. Carbon nanoparticles have a high surface area and are highly reactive, which allows them to interact with the atoms of the host material and modify its properties. The addition of carbon nanoparticles to MgB2 is expected to enhance its superconducting properties by

improving its crystal structure. The addition of carbon nanoparticles to MgB2 is expected to enhance its superconducting properties by several mechanisms. First, the carbon nanoparticles can act as nucleation sites for the formation of MgB2 crystals, promoting the growth of large, well-defined crystals with fewer defects. This can improve the superconducting properties of the material by reducing the number of impurities and defects that can disrupt the flow of electrical current. In addition, the carbon nanoparticles can also modify the electronic structure of MgB2, leading to an increase in the density of states near the Fermi level. This can enhance the superconducting properties of the material by increasing the number of available electronic states that can participate in the superconducting process.

The main aim of this research is to focus on the XRD analysis of pure MgB2 and nano carbon-doped MgB2 superconductor and investigate the effect of nano carbon doping on the crystal structure of MgB2. The XRD patterns of the samples were recorded at room temperature, and the data were analyzed using the standard relation for hexagonal crystal structures of space group p6/mmm. After obtaining the XRD data, we will use specialized software such as X'Pert HighScore Plus to analyze and interpret the data. This software allows us to compare the patterns of pure MgB2 and nano carbon-doped MgB2 to identify any changes in the crystal structure due to carbon doping. The software can also determine the lattice parameters, which are important parameters that describe the crystal structure of a material. We will then plot the XRD patterns of both samples on a graph using the software. The graph will display the intensity of the X-rays diffracted by the sample versus the diffraction angle, which can help us identify the peaks in the patterns. These peaks represent the arrangement of atoms in the crystal structure and can be used to determine the crystal structure and lattice parameters of the material. By comparing the XRD patterns of pure MgB2 and nano carbon-doped MgB2, we can identify any changes in the crystal structure due to carbon doping. These changes may include shifts in the positions of the peaks or changes in the peak widths or intensities. Analyzing these changes can help us understand the influence of carbon doping on the crystal structure and superconducting properties of MgB2.

THEORY

Magnesium diboride (MgB2) is a grey colored, water-insoluble solid inorganic compound. It is a superconductor at a relatively high temperature of 39°K (-234°C). The superconducting mechanism of MgB2 is primarily described by the BCS (Bardeen-Cooper-Schrieffer) theory. In MgB2, magnesium has an ionic bond with boron atom. The synthesis of MgB2 was first reported in 1953, and its crystal structure was confirmed at that time. The simplest synthesis method involves the high-temperature reaction between boron and magnesium powders, with the formation beginning at 650°C. The melting point of MgB2 is relatively high, at 830°C.

The crystal structure of MgB2 is hexagonal and belongs to the AlB2 type crystal structure with a p6/mmm space group, which is common among diborides. The boron atoms form a graphite-like honeycomb network, and the magnesium atoms are located at the pores of these hexagons. Each magnesium atom located at the center of the hexagon formed by boron donates its electron to the B planes. The lattice parameters of MgB2 are a = 0.3084 nm and c = 0.3524 nm, and the atomic distances are as follows: B-B intralayer = 0.1780 nm, Mg-Mg intralayer = 0.3084 nm, Mg-Mg interlayer = 0.3524 nm, and Mg-B interlayer = 0.25 nm. Notably, the in-plane B-B distance is almost half that of the inter-plane B-B distance.

The unique crystal structure of MgB2 is the key to its superconducting properties. The hexagonal structure of MgB2 allows for strong in-plane covalent bonding between boron atoms, which is crucial for superconductivity. The lattice vibrations in the boron planes also play a significant role in MgB2's superconductivity, and these vibrations are sensitive to impurities and defects in the crystal structure. Additionally, the presence of magnesium in the interlayer sites enhances the interlayer electron coupling, leading to a higher transition temperature. The crystal structure of MgB2 is, therefore, a crucial factor that determines its superconducting properties, and understanding it is essential for further research in the field.

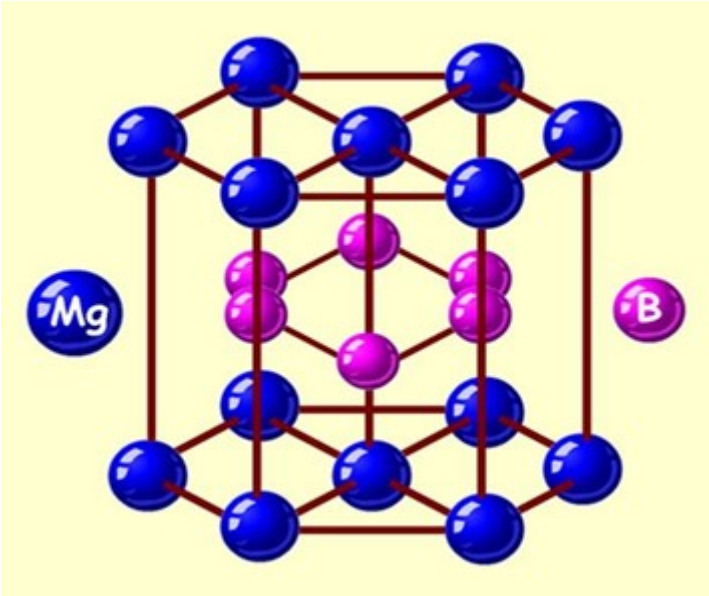


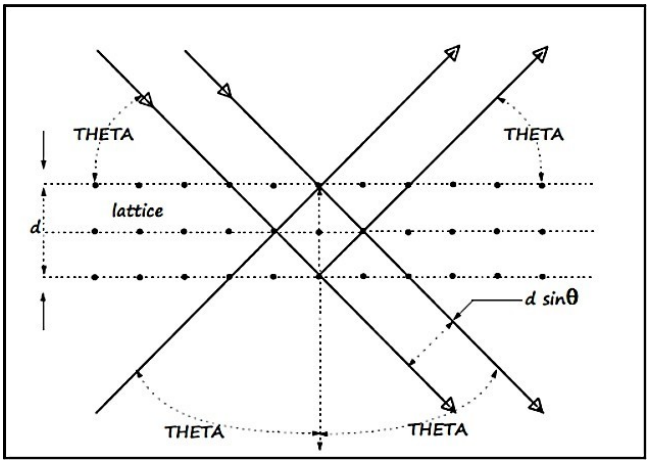
Fig 1 – Structure of MgB

X-ray diffraction (XRD) is a technique used to determine the crystal structure of materials. When monochromatic X-rays are incident on a crystal, the X-rays undergo reflection, producing a diffraction pattern. This diffraction pattern is unique to the crystal structure of the material and can be used to determine the position of the atoms within the crystal. The angle of incidence of the X-ray beam and the distance between atomic layers in the crystal are critical factors that affect the diffraction pattern. The Bragg equation, n = 2d sinθ, explains the relationship between these factors. The variable d is the distance between atomic layers in the crystal, and the variable lambda ( ) is the wavelength of the incident X-ray beam. The angle of incidence (theta, θ) is the angle between the incident X-ray beam and the atomic planes in the crystal. The variable n is an integer that gives the order of reflection, where the reflection corresponding to n=1,2,3 etc. are referred to as first order, second order, third order, etc.

The Bragg equation is a fundamental equation in XRD, and it plays a critical role in the analysis of XRD data. The equation shows that the angle of incidence required for reflection is dependent on the interatomic spacing in the crystal. The diffraction pattern produced by the crystal is a series of peaks, and the position and intensity of these peaks are used to determine the crystal structure. The positions of the peaks are related to the interatomic spacing in the crystal, and the intensity of the peaks is related to the number of atoms within

the unit cell of the crystal.

The XRD pattern is analyzed using specialized software that compares the experimental data with a database of known crystal structures. The software matches the positions of the peaks in the experimental data to the expected positions for a specific crystal structure. The intensity of the peaks is also analyzed to determine the number of atoms within the unit cell. The XRD analysis provides critical information about the crystal structure of the material, including the lattice parameters, interatomic spacing, and atomic positions. This information is essential in the development of new materials and the optimization of material properties.



When X-rays are incident on a crystal, they interact with the electrons and nuclei of the atoms in the crystal lattice. This interaction results in the X-rays being scattered in different directions. The pattern of scattered X-rays is then recorded on a detector, which produces an X-ray diffraction pattern. The X-ray diffraction pattern contains information about the crystal structure of the material, such as the spacing between the planes of atoms in the crystal lattice.

The d values of selected peaks from the X-ray diffraction pattern are used to calculate the lattice parameters of the crystal structure of the material. The lattice parameters are the lengths of the edges of the unit cell that contains the atoms of the crystal lattice. In the case of MgB2, the crystal structure is hexagonal and has a space group of p6/mmm. The lattice parameters a and c are calculated using the relation :

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

Where, d is the interplanar spacing of the planes of atoms in the crystal lattice, and (h k l) are the Miller indices of the planes.

Miller indices are a set of three integers that are used to describe the orientation and spacing of crystal lattice planes in a crystalline material. They are determined by the positions of the lattice points and the orientation of the crystal lattice. The Miller indices are named after William Hallowes Miller, who introduced them in 1839. The Miller indices are written as (h k l) and are enclosed in square brackets [h k l]. The Miller indices represent the reciprocal values of the intercepts made by the plane on the crystallographic axes. The values of h, k, and l can be any integer, and they represent the number of unit cell lengths that the plane intercepts along the x, y, and z axes, respectively. The Miller indices are important for understanding the crystal structure of materials and for analyzing X-ray diffraction patterns.

The Miller indices represent the reciprocal of the intercepts of a crystal plane with the crystallographic axes. They indicate the orientation of the crystal plane with respect to the crystallographic axes, and they provide a convenient way to label and describe the various planes in a crystal lattice. To determine the Miller indices of a crystal plane, one identifies the intercepts of the plane with the three crystallographic axes and takes the reciprocals of those intercepts. For example, consider a crystal lattice with three axes, a, b, and c, intersecting at right angles. If a plane intersects the a-axis at a distance of 2 units, the b-axis at a distance of 3 units, and the c-axis at a distance of 4 units, then the Miller indices of that plane are (1/2, 1/3, 1/4). The reciprocals are then multiplied by a common denominator, such that the resulting indices are integers. The resulting set of integers represents the Miller indices of the crystal plane. In this example, multiplying the reciprocals by 12 gives the Miller indices of (6, 4, 3).

Miller indices are important in materials science and engineering, as they are used to describe the structure and properties of crystalline materials. Crystalline materials have a repeating pattern of atoms or molecules that forms a crystal lattice. The properties of the crystal lattice depend on the arrangement of atoms or molecules within the lattice, as well as the orientation of the crystal planes with respect to the crystallographic axes. The Miller indices provide a way to describe this orientation and spacing.

In materials science and engineering, Miller indices are often used to describe the direction and planes of atomic bonds, defects, and crystal growth. For example, in crystal growth, the orientation of crystal planes with respect to the substrate can affect the quality of the crystal. By controlling the orientation of crystal planes, it is possible to grow high-quality crystals with specific properties. Similarly, defects in crystals, such as dislocations or grain boundaries, can affect the properties of the material. The Miller indices can be used to describe the orientation and position of these defects within the crystal lattice.

Miller indices are also used in X-ray diffraction experiments to identify the crystal structure of materials. X-ray diffraction is a technique used to study the structure of materials by analyzing the way X-rays are scattered by the atoms in a crystal. When X-rays are scattered by a crystal, they form a diffraction pattern that can be used to determine the spacing of the atoms within the crystal lattice. The spacing of the atoms can be determined by measuring the angles and intensities of the diffracted X-rays. By analyzing the diffraction pattern, the crystal structure can be identified using the Miller indices to describe the spacing of the crystal planes.

EXPERIMENTAL AND SETUP

The synthesis process used is the Powder In Sealed Tube method, which involves using stainless steel tubes as the container for synthesis. One end of the tube is pressed uniaxially using a hydraulic press to create a tape shape. Stoichiometric amounts of magnesium and boron powders are accurately weighed using an electronic balance and mixed using an agate mortar and pestle. The resulting powder mixture is densely packed through the open end of the pressed stainless steel tube and pressed again. The other end of the tube is sealed with arc welding to prevent the escape of volatile Mg vapor during the heat treatment. The samples are then heat-treated directly in air at temperatures ranging from 600 to 900°C with a ramp rate of 5°C/min, followed by furnace cooling. To obtain bar-shaped MgB2 cores, the authors extract them by grinding the edges of the samples and mechanically peeling off the stainless steel sheath for structural characterization.

After synthesizing the samples, the authors use X-ray powder diffraction to identify the phases and characterize the structure of the material. X-ray powder diffraction is a widely used technique for phase identification of crystalline materials, which provides information about the lattice parameters, grain size, and strain of the sample. In this study, the authors use a Philips X'pert Pro (PW 3040/60) X-ray diffractometer with CuKa radiation and a proprietary detector called X'Celerator. This system has fully automated operation and data acquisition with programmable slits used to limit the X-ray beam to the specified sample area. The samples are ground thoroughly into fine powder and filled in standard sample holders. XRD patterns are obtained by scanning the samples from 200 to 800 (2θ values) with a step size of less than 0.020. The tube voltage and current are set to 40 kV and 30 mA, respectively, and most scans take about 20 minutes. The recorded XRD data are then analyzed for phase identification.

Lattice parameters were calculated for the hexagonal crystal structure of space group p6/mmm using the relation:

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

Here, the left-hand side of the equation represents a unit called "inverse square distance," which is commonly used in physics to describe how much the strength of a force or field will decrease as you move away from its source. The right-hand side of the equation involves several parameters:

- h, k, and l are the Miller indices of a crystal plane. These indices describe the orientation of the plane relative to the crystal lattice.
- a is the length of the unit cell edge along a particular crystallographic direction.
- c is the distance between adjacent planes of atoms within the crystal.

This equation is derived from the Bragg equation, which relates the wavelength of light (λ), the distance between the slits in the grating (d), the angle at which the light diffracts (θ), and the order of the diffraction (n):

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

The Bragg equation describes how X-rays or other forms of electromagnetic radiation can be used to study the atomic structure of a crystal. When a beam of X-rays is incident on a crystal, it is diffracted by the atomic planes within the crystal, and the resulting diffraction pattern can be analyzed to determine the crystal's structure. The Miller indices of the planes that cause the diffraction can be obtained by using the Bragg equation and the equation for interplanar spacing.

Program

The program described is a powerful mathematical problem-solving tool that uses Python as its programming language. It is specifically designed to solve complex equations that involve multiple variables and can provide a final solution to the problem based on user input. This program is ideal for scientists and researchers who need to solve complex equations quickly and efficiently. The program takes input values such as h1, k1, l1, d1, h2, k2, l2, and d2 from the user. These values represent different variables in the equation that needs to be solved. Once these inputs are provided, the program goes through a series of calculations to determine the values of other variables, such as c1, a1, b1, c2, a2, and b2.

The first step in the program is to calculate the values of c1, a1, and b1 based on the input values. These calculations are based on specific equations that are related to the input values. Similarly, the program calculates c2, a2, and b2 based on the input values for h2, k2, l2, and d2. Once all the necessary variables have been calculated, the program then solves two equations to find the values of x and y. These equations are typically complex and require a high level of mathematical knowledge to solve them manually. However, since the program is designed to automate this process, it can quickly provide a solution to these equations. Finally, the program uses the solutions obtained for x and y to calculate the values of a and b, which are key components of the overall equation and need to be determined before the final solution can be reached.

The program also provides a means for plotting and analyzing data. The program takes in experimental data and then plots it using specialized software designed for this purpose. Once the data has been plotted, the program can perform various analyses on it to determine important features and characteristics. This analysis can be used to draw conclusions about the data and to make predictions about future experiments.

The program is an essential tool for researchers who need to quickly and efficiently analyze large amounts data.

```python
h1 = float(input("Enter the value of h1: "))
k1 = float(input("Enter the value of k1: "))
l1 = float(input("Enter the value of l1: "))
d_1 = float(input("Enter the value of d_1: "))

d1 = d_1*(10**-10)

h2 = float(input("Enter the value of h2: "))
k2 = float(input("Enter the value of k2: "))
l2 = float(input("Enter the value of l2: "))
d_2 = float(input("Enter the value of d_2: "))

d2 = d_2*(10**-10)

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

print("The solution is x = ", x, " y = ", y)

a = x ** -0.5
b = y ** -0.5

print("The solution is a = ", a, " b = ", b)
```

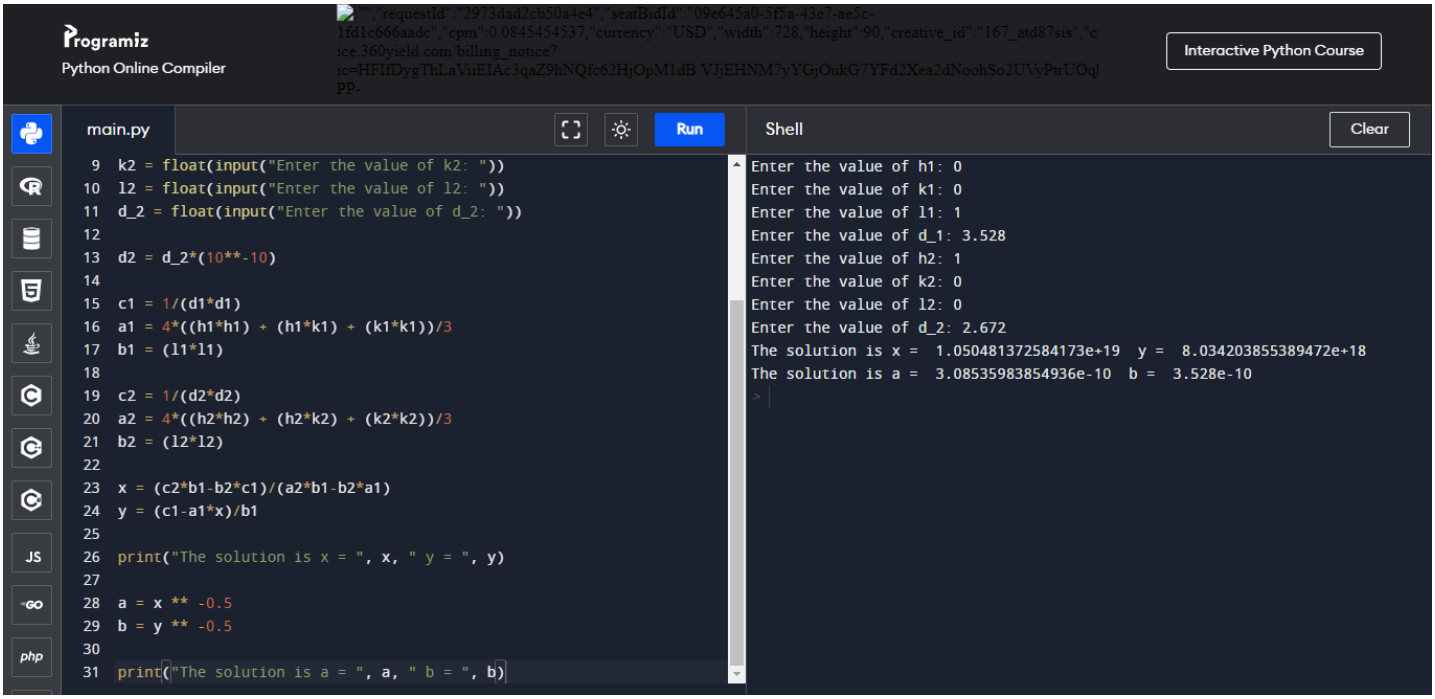
The purity of materials is an important aspect of material science research. In this project, we aim to compare the purity of pure and doped MgB2 samples using X-ray powder diffraction (XRD) data. To accomplish this, we have developed a Python program that can process the XRD data and provide a detailed analysis of the samples' purity. The program allows for a quantitative comparison of the peak intensities between the pure and doped samples, which can indicate the presence of impurities in the doped sample.

Why use Python for this project:

Python is a widely used programming language in scientific research, and for good reason. Its versatility and ease of use make it an ideal tool for data analysis and visualization. Here are some reasons why we chose to use Python for this project :

- Open-source: Python is an open-source language, meaning that it is freely available for use and modification. This makes it an accessible tool for researchers who may not have access to expensive proprietary software.
- Python is a high-level, interpreted programming language that is widely used for a variety of applications. One of the most appealing features of Python is its simplicity and ease of use. The language is designed to be intuitive and easy to understand, making it an excellent choice for beginners and experienced programmers alike.
- Python's syntax is straightforward and easy to read, which allows developers to focus on problem-solving rather than worrying about complex syntax rules. Additionally, Python comes with a vast library of built-in functions and modules that can be used to extend its functionality and streamline the development process.
- Python is also highly versatile, which makes it an excellent choice for a wide range of projects. The language is used for web development, scientific computing, data analysis, machine learning, and more. Python's versatility is due in part to its ability to interface with other languages, making it easy to incorporate code written in other languages into a Python project.

SAMPLE OUTPUT



Demonstration of the program output for MgB2 polycrystalline sample. Using this snippet, you can easily determine the lattice parameters "a" and "c". Later, these values can be compared with those of doped MgB2 compounds. Please note that this is just a sample output image for demonstration purposes.

Observations

INTENSITY VS 2 THETA VALUE FROM EXPERIMENT:

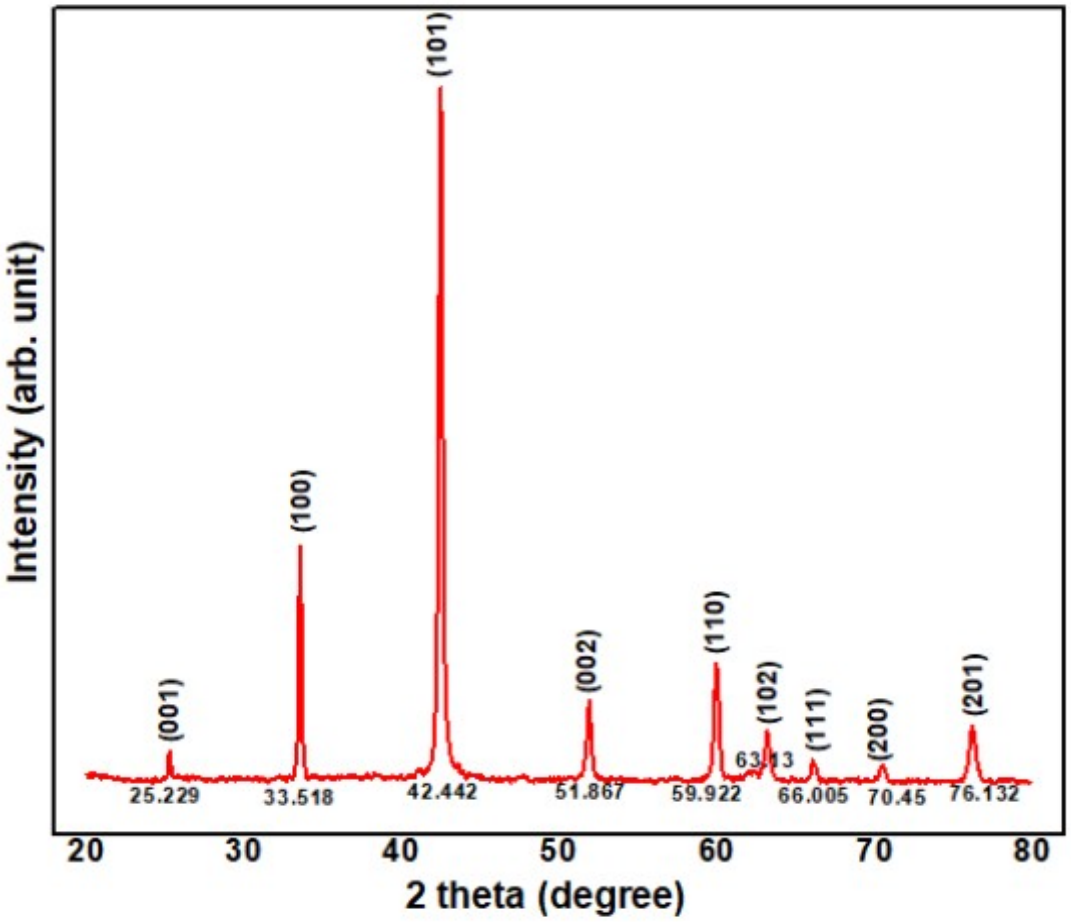
Angle, 2θ	Intensity	Angle, 2θ	Intensity	Angle, 2θ	Intensity	Angle, 2θ	Intensity
20.01536	12.05	26.19457	8.558	32.37378	8.98158	38.55298	11.54627
20.1971	11.0785	26.37631	10.46349	32.55552	9.49572	38.73472	9.11964
20.37884	10.53134	26.55805	8.38489	32.73726	6.97678	38.91647	7.67872
20.56058	12.60264	26.73979	10.12393	32.919	9.83463	39.09821	10.21562
20.74233	11.74484	26.92153	7.64471	33.10074	9.01995	39.27995	8.35522
20.92407	8.6562	27.10327	10.12509	33.28248	29.25407	39.46169	10.11182
21.10581	10.94873	27.28502	7.52602	33.46422	180.7853	39.64343	9.06933
21.28755	11.12463	27.46676	6.59745	33.64596	120.1825	39.82517	9.44083
21.46929	9.9796	27.6485	5.43367	33.82771	22.40776	40.00691	9.03807
21.65103	10.7409	27.83024	7.99161	34.00945	7.02974	40.18866	7.72071
21.83277	8.33949	28.01198	6.54536	34.19119	10.1914	40.3704	11.68499
22.01452	9.54272	28.19372	6.26799	34.37293	10.14975	40.55214	11.09881
22.19626	7.7325	28.37546	7.03016	34.55467	10.53112	40.73388	9.74879
22.378	6.97959	28.55721	8.56718	34.73641	7.29985	40.91562	15.58004
22.55974	7.52705	28.73895	6.66936	34.91815	9.02016	41.09736	17.77812
22.74148	6.36288	28.92069	6.57539	35.0999	8.73539	41.2791	16.09719
22.92322	5.93871	29.10243	7.81423	35.28164	10.18194	41.46084	16.9658
23.10496	6.59892	29.28417	8.50511	35.46338	8.27204	41.64259	18.16229
23.28671	8.09382	29.46591	6.86404	35.64512	8.99191	41.82433	25.22479
23.46845	6.18853	29.64765	7.54354	35.82686	7.37588	42.00607	44.27759
23.65019	4.9665	29.8294	7.05063	36.0086	9.33563	42.18781	145.042
23.83193	6.69932	30.01114	7.22731	36.19034	10.96955	42.36955	605.2514
24.01367	6.42405	30.19288	9.65175	36.37209	10.51922	42.55129	460.7911
24.19541	4.21201	30.37462	7.75897	36.55383	10.37547	42.73303	111.2352
24.37715	8.66128	30.55636	6.2364	36.73557	10.77384	42.91478	51.0638
24.55889	6.44712	30.7381	8.63637	36.91731	10.46737	43.09652	30.96177
24.74064	7.80108	30.91984	5.33878	37.09905	9.21423	43.27826	21.14945
24.92238	8.80161	31.10159	9.43587	37.28079	8.68201	43.46	19.73571
25.10412	11.84724	31.28333	6.59369	37.46253	9.11769	43.64174	18.35549
25.28586	32.02981	31.46507	5.11664	37.64428	10.28516	43.82348	16.33176
25.4676	9.7673	31.64681	8.47995	37.82602	12.79847	44.00522	10.76837
25.64934	9.4653	31.82855	7.69299	38.00776	9.88973	44.18697	12.63673
25.83108	11.63577	32.01029	9.81539	38.1895	13.57591	44.36871	11.08656
26.01283	9.92299	32.19203	9.34125	38.37124	12.59898	44.55045	11.46588

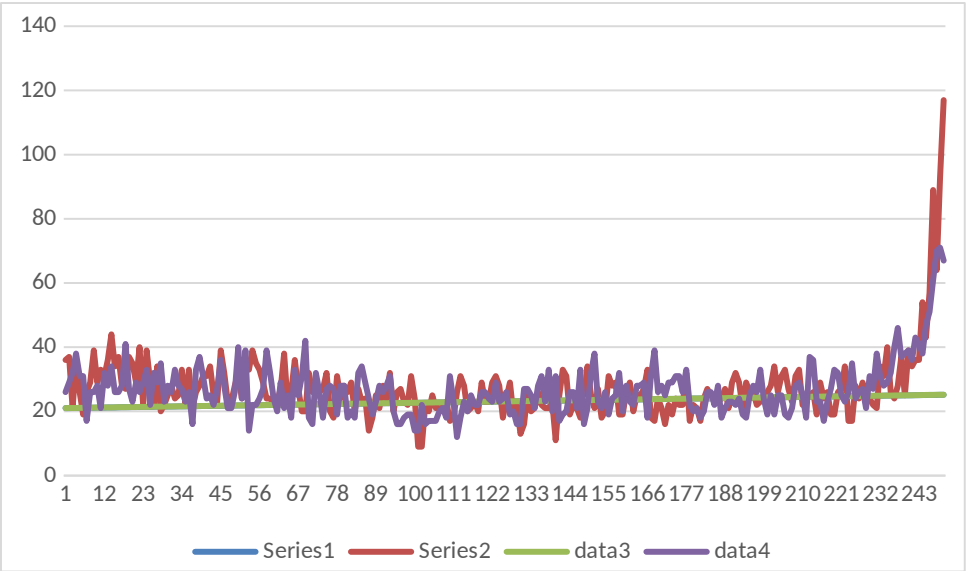
Angle, 2θ	Intensity	Angle, 2θ	Intensity	Angle, 2θ	Intensity	Angle, 2θ	Intensity
44.73219	10.69099	50.9114	7.53956	57.09061	7.83378	63.26981	40.23223
44.91393	7.66301	51.09314	8.59701	57.27235	10.2735	63.45155	19.92002
45.09567	8.75661	51.27488	12.27558	57.45409	7.9272	63.6333	9.58767
45.27741	7.24839	51.45662	16.75792	57.63583	7.03521	63.81504	7.65112
45.45916	7.52957	51.63836	34.95558	57.81757	5.19119	63.99678	6.68003
45.6409	8.47157	51.8201	80.52117	57.99931	6.35408	64.17852	6.54503
45.82264	9.02081	52.00185	46.56433	58.18105	6.15871	64.36026	5.85966
46.00438	6.05281	52.18359	15.9297	58.3628	7.11932	64.542	4.4145
46.18612	9.37921	52.36533	11.89197	58.54454	6.35802	64.72374	7.71985
46.36786	6.79066	52.54707	8.01711	58.72628	6.29341	64.90549	6.26631
46.5496	7.60137	52.72881	8.96765	58.90802	6.14279	65.08723	6.25528
46.73135	9.55435	52.91055	6.68994	59.08976	7.00066	65.26897	7.44468
46.91309	5.85048	53.09229	5.66852	59.2715	10.19122	65.45071	5.82423
47.09483	6.73464	53.27404	9.51292	59.45324	13.75194	65.63245	7.28662
47.27657	8.90758	53.45578	6.93974	59.63498	29.35337	65.81419	9.26894
47.45831	9.11456	53.63752	6.86782	59.81673	93.76393	65.99593	25.88023
47.64005	10.61418	53.81926	9.35358	59.99847	108.766	66.17768	21.02769
47.82179	9.16378	54.001	6.87593	60.18021	42.96075	66.35942	11.59359
48.00354	7.30596	54.18274	5.19289	60.36195	11.68759	66.54116	4.99725
48.18528	6.13092	54.36448	7.14211	60.54369	9.50152	66.7229	5.72755
48.36702	5.79083	54.54623	6.1938	60.72543	9.69767	66.90464	3.57266
48.54876	7.26627	54.72797	5.60427	60.90717	7.48824	67.08638	8.26954
48.7305	6.44821	54.90971	7.13849	61.08892	9.79756	67.26812	7.00193
48.91224	6.41808	55.09145	6.13062	61.27066	7.68148	67.44986	6.76072
49.09398	6.37663	55.27319	5.12331	61.4524	10.79023	67.63161	6.09606
49.27573	7.48664	55.45493	6.51564	61.63414	9.59742	67.81335	3.90129
49.45747	6.00411	55.63667	6.64432	61.81588	12.04344	67.99509	5.50153
49.63921	8.1455	55.81842	6.00117	61.99762	14.86063	68.17683	7.56227
49.82095	8.41281	56.00016	5.37048	62.17936	13.36073	68.35857	7.08742
50.00269	5.86257	56.1819	6.05182	62.36111	15.02356	68.54031	7.38721
50.18443	7.72026	56.36364	8.12911	62.54285	11.85362	68.72205	6.56721
50.36617	7.43303	56.54538	6.85024	62.72459	16.82453	68.9038	8.7524
50.54791	9.51576	56.72712	6.34068	62.90633	25.75982	69.08554	3.44176
50.72966	9.03183	56.90886	8.13813	63.08807	51.11885	69.26728	5.27859

Angle, 2θ	Intensity	Angle, 2θ	Intensity
69.44902	6.38311	75.62823	9.49252
69.63076	5.67896	75.80997	19.12866

69.8125	5.55219	75.99171	42.42973
69.99424	9.28336	76.17345	61.13372
70.17599	9.79443	76.35519	39.95296
70.35773	19.08171	76.53693	17.46918
70.53947	18.92164	76.71868	9.09106
70.72121	9.35526	76.90042	4.81196
70.90295	5.20619	77.08216	5.74654
71.08469	3.99525	77.2639	6.74971
71.26643	6.10427	77.44564	5.82917
71.44818	5.46798	77.62738	4.12679
71.62992	4.42202	77.80912	6.84042
71.81166	5.73868	77.99087	5.86884
71.9934	4.28955	78.17261	6.99879
72.17514	7.33725	78.35435	7.91493
72.35688	6.85655	78.53609	7.00064
72.53862	5.68327	78.71783	7.74344
72.72037	7.59305	78.89957	4.70147
72.90211	5.24181	79.08131	4.90555
73.08385	5.44917	79.26306	5.90443
73.26559	6.29083	79.4448	5.51726
73.44733	5.70595	79.62654	4.95063
73.62907	5.9815	79.80828	4.13

After conducting the X-ray powder diffraction technique, we use the obtained data to create a graph that displays the results:


Intensity (arb. unit)
(001)
(100)
(101)
(002)
(110)
(102)
(111)
(200)
(201)
25.229
33.518
42.442
51.867
59.922
63.13
66.005
70.45
76.132
20
30
40
50
60
70
80
2 theta (degree)



λ =1.541 Å *Using Braggs law*,

$d = (n \lambda) / (2 \sin\theta)$; $n = 1$ (*First order*)

From the graphical data:

λ (Å)	(h k l)	2θ (º)	Θ (º)	d=(nλ)/2sinθ (Å)
1.541	(001)	25.229	12.614	d1 = 3.528
	(100)	33.518	16.759	d2 = 2.672
	(101)	42.442	21.221	d3 = 2.128
	(022)	51.867	25.933	d4 = 1.761
	(110)	59.922	29.961	d5 = 1.542
	(102)	63.13	31.565	d6 = 1.471
	(111)	66.005	33.002	d7 = 1.414
	(200)	70.45	35.225	d8 = 1.335
	(201)	76.132	38.066	d9 = 1.249

TABLE 1

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

To determine the values of hkl from the X-ray powder diffraction graph, we first identify the peaks and measure their corresponding angles, denoted by theta (θ). Using Bragg's law, we can then calculate the wavelength (λ) of the X-ray radiation diffracted by the crystal. Finally, we assign the values of hkl based on the known crystal structure and Miller indices for each corresponding peak, and record these values in the "observation" column.

Result

(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=3.528	$1/d1^2 = 1/c^2$	-	3.528
(100)	d2=2.672	$1/d2^2 = 4/3a^2$	3.085	-
(101)	d3=2.128	$1/d3^2 = (4/3a^2) + (1/c^2)$	-	-
(002)	d4=1.761	$1/d4^2 = 4/c^2$	-	3.522
(110)	d5=1.542	$1/d5^2 = 4/a^2$	3.084	-
(102)	d6=1.471	$1/d6^2 = (4/3a^2) + (4/c^2)$	-	-
(111)	d7=1.414	$1/d7^2 = (4/a^2) + (1/c^2)$	-	-
(200)	d8=1.335	$1/d8^2 = 16/3a^2$	3.083	
(201)	d9=1.249	$1/d9^2 = (16/3a^2) + (1/c^2)$	-	-

TABLE 2

Practical Application

Superconductivity is the phenomenon of zero electrical resistance and the expulsion of magnetic fields in certain materials when they are cooled below a certain critical temperature. This property of superconductors has many practical applications in various fields of science and technology.

Here are some of the applications of superconductivity:

1. MRI is a non-invasive medical imaging method that utilizes powerful magnetic fields to produce detailed images of the body. The technique employs superconducting magnets, which can generate magnetic fields that are up to 60,000 times stronger than the Earth's magnetic field. The implementation of superconducting magnets in MRI technology has considerably improved the precision and effectiveness of medical imaging.

2. Superconducting magnets are utilized in particle accelerators to generate robust magnetic fields that direct and concentrate the accelerated particles. These magnets also aid in steering the particles and managing their path.

3. The application of superconducting materials in power transmission systems can enhance the energy efficiency of electrical power transmission. As electrical current flows through a conductor, some of its energy is dissipated in the form of heat. However, since superconducting materials possess zero electrical resistance, no energy is dissipated as heat when electrical current flows through them. Consequently, superconducting materials are an optimal choice for use in power transmission cables.

4. The capacity of superconducting materials to retain electrical energy in magnetic fields permits prompt discharge of energy when necessary. This property makes superconducting energy storage systems well-suited for applications where swift energy discharge is necessary, such as in power grids.

5. The implementation of superconducting materials can generate robust magnetic fields capable of levitating objects. Maglev trains utilize this technology to float above the tracks and achieve high speeds through magnetic levitation.

Let's explore the uses of MgBr2.

MgBr2, a crystalline white substance, has diverse applications across numerous industries. The primary applications of MgBr2 include its use as a catalyst in organic synthesis and as a flame retardant in plastics and textiles. MgBr2 is also used in the production of magnesium metal and in the oil and gas industry as a completion fluid.

MgBr2 plays a crucial role in the production of magnesium metal, a valuable material utilized in numerous industries such as aerospace, automotive, and electronics. MgBr2 is employed as a precursor for magnesium metal production, which involves its extraction via electrolysis.

CONCLUSION

The results of our analysis showed that the doping of carbon had a significant effect on the lattice parameters of the MgB2 superconductor. The value of the lattice parameter a increased while the value of c decreased, compared to the undoped MgB2. This suggests that the carbon atoms have replaced some of the boron atoms in the crystal structure, causing a distortion in the lattice. The distortion caused by the carbon doping can potentially improve the electronic and magnetic properties of the material, leading to better superconducting properties.

The use of a Python program for analyzing the XRD data provided several advantages over manual methods. The program enabled fast and precise determination of peak positions and intensities, as well as calculation of lattice parameters, eliminating the possibility of human error. Furthermore, the program can be easily modified to analyze data from other materials and perform more complex calculations.

In conclusion, this project demonstrates the importance of XRD analysis in understanding the crystal structure of materials, particularly superconductors. The use of a Python program for analyzing XRD data provides a powerful and efficient tool for researchers in this field. The results of our analysis of the nano carbon doped MgB2 superconductor showed promising changes in the lattice parameters, which could potentially lead to improvements in its superconducting properties. This opens up new avenues for research in the field of superconductivity, and further exploration of the effects of carbon doping on MgB2 and other superconductors.

Reference

- *G. Grasso, A. Malagoli, C. Ferdeghini, S. Roncallo, V. Braccini and A. S. Siri, Appl. Phys. Lett.*
- *Neson Varghese, K. Vinod, S. Rahul, K. M. Devadas, Syju Thomas, S. Pradhan and U. Syamaprasad, J. Appl. Phys.*
- *G. K. Williamson and W. H. Hall, Acta Materillia*